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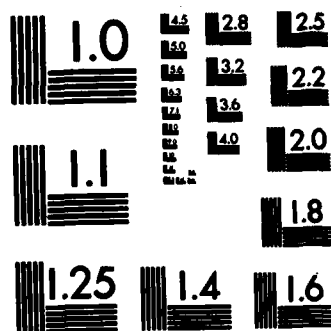
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HOW TO EVALUATE AND SYNTHESIZE LITERATURE DATA ON PHYSICAL PROPERTIES

by

C. Y. Ho and Y. S. Touloukian



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HOW TO EVALUATE AND SYNTHESIZE LITERATURE DATA ON PHYSICAL PROPERTIES

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I. INTRODUCTION

Owing to the difficulties encountered in the accurate measurement of properties of materials and in the adequate characterization of test specimens, especially solids, the property data recorded in the scientific and technical literature are often conflicting, widely diverging, and subject to large uncertainty. Indiscriminate use of literature data for engineering and design calculations without knowing their reliability is dangerous and may cause inefficiency or product failure, which at times can be disastrous. Consequently, only critically evaluated reference data should be used for such and other purposes. It is, therefore, very important to critically evaluate and analyze the available data and information, to give judgment on the reliability and accuracy of the data, and to generate recommended reference data.

The Center for Information and Numerical Data Analysis and Synthesis (CINDAS) at Purdue University is a specialized National Center for the identification, compilation, critical evaluation, analysis and synthesis of numerical data on the physical properties of materials with the aim of generating recommended reference data for nation-wide dissemination. Thus the generation of reference data on the physical properties of materials discussed herein is the very mission of CINDAS. CINDAS is a component of the U.S. National Standard Reference Data System (NSRDS) under the auspices of the National Bureau of Standards and it also operates the Thermophysical and Electronic Properties Information Analysis Center (TEPLAC) for the U.S. Department of Defense.

CINDAS covers fourteen thermophysical properties and twenty-two electronic, electrical, magnetic, and optical properties of nearly all materials in all physical states and at all temperatures and pressures. Over the past twenty-three years the staff members at CINDAS have compiled more than 100,000 sets of experimental data from the world literature and have continuously been performing data evaluation, correlation, analysis, and synthesis to generate recommended reference data for meeting the needs of the Nation.

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In the following sections the methodology of critical evaluation, correlation, analysis, and synthesis of physical property data will be discussed and the generation of recommended reference data will be illustrated with examples covering thermal, electrical, thermoelectric, and optical properties of solids. It will show also how this activity brings order out of very chaotic experimental observations. While data evaluation and analysis deal mainly with the validity, reliability, and accuracy of existing experimental data, data synthesis is a process of generating a full field of new data based on limited fragmentary experimental information coupled with a knowledge of the theory. It is important to note that reference data, though much useful and reliable, are generated at a very small fraction of the cost and time required for producing the experimental data.

II. DATA EVALUATION, ANALYSIS, AND SYNTHESIS AND GENERATION OF REFERENCE DATA

Reference data are generated through critical evaluation, correlation, analysis, and synthesis of the available experimental data compiled from all sources. The procedure involves critical evaluation of the validity of the available data and related information, judgment on the reliability and accuracy of the data, resolution and reconciliation of disagreements in conflicting data, correlation of data in terms of various controlling parameters (sometimes in reduced forms using the principle of corresponding states), curve fitting with theoretical or empirical equations, synthesis of the often fragmentary data to generate a fuller range of coverage of internally consistent values, comparison of the resulting recommended values with theoretical predictions or with results derived from theoretical relationships or from generalized empirical correlations, etc.

Considering the thermal conductivity data, for example, in the critical evaluation of the validity and reliability of a particular set of experimental data, the temperature dependence of the property data is examined, and any unusual dependence or anomaly is carefully investigated. The experimental technique is reviewed to see whether the actual boundary conditions in the measurement agreed with those assumed in the theoretical model used to define the property. It is ascertained whether all the stray heat flows and losses were prevented or minimized and accounted for. Furthermore, the reduction of

the data is examined to see whether all the necessary corrections were appropriately applied, and the estimation of uncertainties is checked to ensure that all the possible sources of error, particularly systematic errors, were considered by the author(s).

Since the primary factor contributing to unreliable and erroneous experimental results is the systematic error in the measurements, experimental data can be judged to be reliable only if all sources of systematic error have been eliminated or minimized and accounted for. Considering the measurement of thermal transport properties such as thermal conductivity, for example, the major sources of systematic error may include at least the following:

- (1) Unsuitable experimental method. In measuring the thermal conductivity of a solid, a number of different methods are best suited for different ranges of temperature and for various classes of materials having different ranges of thermal conductivity values. Thus, a particular method may be preferable to others for a given material and temperature range, and no one method is suitable for all the required conditions of measurement. Therefore, the first thing to look for is whether the author used the most suitable experimental method in his measurement. Because the available experimental facility in each laboratory is limited, at times, one is forced to extend the temperature range of measurement beyond that for which his apparatus was designed, by certain modification of the apparatus. In such cases, accurate results usually cannot be expected.
- (2) Poor experimental technique. There are many pitfalls in each experimental method. To avoid them, the experimenter must employ very sound experimental techniques so that all steps are properly executed. These involve know-how, skill and ingenuity and make the difference between an outstanding experimenter and an ordinary one. These include good overall experimental set-up, refined technique for fabricating and installing the specimen heater so as to minimize heat leakage, technique for installing temperature sensors such as thermocouples so as to assure good thermal contact with the specimen, technique for bringing thermocouple leads away from the specimen along an isotherm and subsequent sound thermal grounding, technique

for good thermal guarding to eliminate stray heat flows, etc. In reading between lines, one may detect whether the author's technique was poor or sound.

- (3) Poor instrumentation and poor sensitivity of measuring circuits, sensors, or devices. For example, thermocouples must be calibrated for accurate interpretation. One should never accept supplier's calibration, which usually is unprecise and often useless. After being installed into the apparatus, the thermocouples should be intercompared or intercalibrated inside the apparatus during the measurement at each temperature to eliminate any intrinsic differences in e.m.f. among the thermocouples or any induced differences in e.m.f. introduced by the cold-working during installation. The potentiometer and other instruments used should, of course, have high sensitivity.
- (4) Mismatch between actual experimental boundary conditions and those assumed in the theoretical model to derive the property value. In thermal conductivity measurement, the heat flow in the specimen is assumed to follow a predetermined pattern, say, either axial or radial. In the case of axial flow, for example, there should be no heat straying normally to the axial direction. Otherwise, the actual experimental boundary conditions will not agree with those assumed in the model. If complete elimination of the traverse heat flow is not possible, it should at least be minimized and evaluated to be accounted for as corrections. Temperature drift is another cause of mismatch of boundary conditions.
- (5) Specimen and/or thermocouple chemical contamination. Specimen and/or thermocouple contamination may result from oxidation or from reaction of the specimen and/or thermocouple with apparatus components or with each other. It occurs especially when the measurement is made at high temperatures, and is a major source of error. One may detect it by simultaneous measurements of the electrical resistivity and thermoelectric power of the specimen if it is an electrical conductor and observing whether there are changes in the measured values of these two properties on thermal cycling. One may also install auxiliary temperature sensors such as resistance thermometers or thermocouples of a different kind for detection.

- (6) Unaccounted-for stray heat flows. Stray heat flows may be heat gains or losses to or from the specimen due to radiation interchange or due to conduction through the surrounding insulation, along the electric leads, along the thermocouple wires and the ceramic insulating tubing or supports. Stray heat flows may be detected by the measurement of a material of known lower thermal conductivity using the same apparatus. Since stray heat flows would have a much stronger effect on the result of measurement on low-conductivity materials, they would reveal themselves clearly in such a calibrating measurement. In connection with apparatus calibrations, there is an urgent need for standard reference materials.
- (7) Incorrect form factor. The form factor relates the observable quantities to the value assigned to the property, and should be known accurately. In measurements at high temperature, the form factor is affected by thermal expansion. Since different experimental methods and apparatus have different form factors, the error in the form factor may be detected by a measurement with an alternate method and intercomparing the results. On the other hand, if a multi-property apparatus is used, any error in the form factor can easily be detected by checking the experimental result of one of the known properties.

Those discussed above, and other possible sources of error, should be carefully considered in critical evaluation of experimental data. These objective criteria are most important in value judgment.

In many cases, however, research papers do not contain adequate information for a data evaluator to perform a truly critical evaluation. In these cases, some other considerations may have to be used for data evaluation. For instance, if several authors' data agree with one another and, more importantly, these were obtained by using different experimental methods, these data are likely to be reliable. However, if the data were observed by means of the same experimental method, even though they all agree, the reliability of the data is still subject to questioning, because they may all suffer from a common, but unknown, source of error. Secondly, if the same apparatus had been used for measurements of other materials and the other results are reliable, and if the

result of measurement on the new material is in the same range, the result for the new material is likely to be reliable. However, if the information given by the author is entirely inadequate to make any value judgment, the data assessment becomes subjective. At times, judgments may be based upon factors and considerations such as the purpose of and the motivation for the measurement, general knowledge of the experimenter, his past performance, the reputation of his laboratory, etc.

In the process of critical evaluation of experimental data outlined above, unreliable and erroneous data are eliminated. The remaining data are then subjected to further analysis and used for data correlation and synthesis. If a number of data sets are available for a well-characterized material, correlation of the data in terms of the affecting parameters may be made. These parameters may include purity, composition, residual electrical resistivity or electrical resistivity ratio (if a metal), density or porosity, hardness, crystal axis orientation, degree of cold working, degree of heat treatment, etc. Applying the principle of corresponding states, reduced property values may be correlated with reduced temperature, pressure, and other reduced parameters. Furthermore, by using theoretical relationships, several properties of the same material may be cross-correlated to check for internal consistency of the data or to estimate property values. For example, data on thermal conductivity, specific heat and density may be combined to compare with thermal diffusivity data measured directly, and data on the viscosity, specific heat, and thermal conductivity of a gas can be correlated with data on the Prandtl number. For a fluid, the property of the saturated liquid can also be correlated with that of the saturated vapor. In data synthesis, the availability of a few reliable experimental data is necessary. If there exists a theory that has been tested and confirmed by reliable data, and thus has proven to be reliable, it can then be used for the generation of new property values or filling data gaps. It is important to note here the difference between a purely theoretical calculation and the data synthesis discussed here. Sometimes semiempirical techniques are also employed to fill data gaps.

If no adequate theory is available that can be used as a guide for the synthesis of fragmentary data, graphical smoothing and synthesis may sometimes be used. In graphical smoothing and synthesis of data for an alloy system, for example, cross-plotting from property data versus temperature to property data

versus composition and vice versa are often used. Smooth curves are drawn which approximate the best fit to the property data versus temperature, and points from the smoothed curves are used to construct property-versus-composition curves for a convenient set of selected temperatures. In the property-versus-composition graph, the families of isotherms are similar and any required smoothing of the data can be done more easily and with greater confidence than when working directly with the property-versus-temperature curves. The points from the resulting smoothed curves are then used to construct property-versus-temperature curves for the selected compositions, and these curves are further smoothed. In the graphical smoothing process it is extremely important that the alloy phase diagrams be frequently consulted and the phase boundaries between solid solutions and/or mechanical mixtures and the boundaries of magnetic transitions be kept in mind, so as to be aware of any possible discontinuity or sudden change of slope of the property curves.

III. SAMPLES OF DISCORDANT EXPERIMENTAL DATA

1. Thermal Conductivity of Titanium Carbide

The scientific and technical literature is full of inaccurate and erroneous data. One example showing disagreement in conflicting data is the thermal conductivity of titanium carbide shown in Figure 1. In this figure the lower data are about 5 times lower than the upper data at 800 K and are about 10 times lower at 1350 K. The lower two sets of data were published by a well-known scientist in 1954 and were obtained by using two completely different experimental methods and confirmed by each other. These lower data were the only data available before 1961, and machine tool designers might have used these erroneous data for years since titanium carbide has been extensively used to make machine tools. One can imagine the consequence of using a 10-times-lower value for designing a machine tool or anything. Since 1961, newer measurements indicate that the thermal conductivity of titanium carbide is actually increasing with temperature, instead of decreasing when the temperature increases as indicated by the lower two sets of data, and the true values are so much higher. It is easy to prove that the lower data are wrong by a simple analysis. The total thermal conductivity, λ , of an electrically conducting material such as titanium carbide consists of two components: an electronic component, λ_e , and a lattice component, λ_g . λ_e may be calculated from electrical resistivity data

and the resulting calculated values for λ_e of titanium carbide are much higher than the lower two sets of data in Figure 1, which are for the total thermal conductivity, λ . Since the whole must be greater than a part, λ must be greater than λ_e . This proves that the lower data, which are for λ but much smaller than λ_e , are impossible.

2. Thermal Conductivity of Platinum + Rhodium Alloy

Another example of conflicting data available from the literature is shown in Figure 2. This is on the thermal conductivity of platinum (60%) + rhodium (40%) alloy. At the lower temperature end, the upper data are higher than the lower data by about 140%. In this case the lower data are correct and the upper data are wrong. To prove that the upper data are wrong is simple. These upper data are much higher than those for pure platinum and are as high as those for pure rhodium, which is utterly impossible for a high alloy of solid solution of platinum and rhodium, because as a function of composition the thermal conductivity of a binary solid-solution alloy system decreases rapidly to a minimum at a certain composition in the middle range. Furthermore, the rapid decrease of thermal conductivity with increasing temperature is also unlikely for a high alloy, that is, the slope of the curve is also wrong.

3. Thermal Conductivity of Gadolinium

Figure 3 shows another type of disagreement in experimental data from the literature. Here the two sets of thermal conductivity data for gadolinium are for the same one piece of specimen measured in the same laboratory which is one of the best known internationally, and published two years apart in 1967 and 1969. The accuracy of curve 1 was stated as within one percent and that of curve 2 as 0.5 percent, though the two curves differ from each other by up to 500 percent at the higher temperature end. These large differences between the two sets of data cannot be attributed to the difference between the specimens because the two data sets are for the same piece of specimen, nor can one judge which laboratory is better because both data sets are from the same laboratory.

4. Thermal Conductivity and Thermal Diffusivity of Tungsten

Figure 4 presents the experimental data and the recommended values for the thermal conductivity of tungsten and shows that most of the experimental data

are erroneous, conflicting, and widely diverging. It has been estimated that the cost of experimental research is about \$50,000 per published research paper. Since the number of published papers reporting experimental results on the thermal conductivity of tungsten is more than 100, a total of over \$5,000,000 research funds had been spent to produce the confusion of experimental data shown in Figure 4. On the other hand, one can see the obvious discrepancy only when both good and bad data are at hand. In the search of literature for data, if one obtains only the portion of bad data, he won't be able to make meaningful comparison. This points out further the importance of an information analysis center such as TEPIAC/CINDAS who systematically and comprehensively collects all the available data. If one obtains, for example, only the several lower or higher curves of Figure 4 in his search of literature for the thermal conductivity of tungsten, no meaningful comparison can be made at all. In this figure erroneous data are everywhere and they differ from each other in the extreme by over 300 percent. It is convincing by observing Figure 4 that the true values of the thermal conductivity of tungsten were not known until TEPIAC/CINDAS critically evaluated the discordant experimental data and generated the recommended reference values.

The experimental data and the recommended values for the thermal diffusivity of tungsten are shown in Figure 5. It shows that the lower three sets of data are utterly erroneous, being about five times too low. The recommended curve shown in the figure generated in 1971 by TEPIAC/CINDAS not only gives the correct thermal diffusivity values for tungsten but also covers a full range temperature, going far beyond the limited range covered by the discordant experimental data.

5. Thermal Conductivity of Nickel

In Figure 6 the three sets of data on the thermal conductivity of nickel with data set numbers 36, 37, and 66 have extremely high slopes, and yet these are some of the most recent data published in internationally well-known scientific journals. In fact, the data of data set 66, which have an incredible nearly vertical slope, are the most recent of all the data shown in Figure 6. One might wonder why the editors of internationally reputable scientific journals would allow such erroneous data to appear in their journals to pollute the scientific and technical information.

6. Errors Found in Generally Accepted, Widely Used Reference Sources

Not only cases of discordant experimental data showing lack of agreement are numerous, but even reference values published in well-known reference books and handbooks can be very much in error. For example, let us examine a widely used and much consulted reference work: the Metals Handbook. The Eighth Edition of it was published in 1961 and the latest Ninth Edition in 1979.

In the 1961 Edition of the Metals Handbook, thermal conductivity values are given for 64 elements and some other materials mainly for near room temperature. Many of these values are identical with those given in the Seventh Edition published in 1948, which covers 45 elements. Of the 64 values given in the 1961 Edition for the 64 elements near room temperature, 18 are in error by over 20 percent, 11 of the 18 are in error by over 30 percent, 8 of the 11 are in error by over 40 percent, and 5 of the 8 are in error by over 50 percent. There is an interesting story about the value given for the thermal conductivity of indium which is in error the most; the correct value is greater by a factor of 3.4. Although the thermal conductivity of indium at room temperature and above was not measured until 1962, the room-temperature value for the thermal conductivity of indium had been listed since the 1936 (Fifth) Edition of the Metals Handbook, and the same value had appeared also in a 1937 Russian handbook entitled "Compilation of Physical Constants" and in a number of other Russian and American handbooks and reference books published subsequently. The original source of this erroneous value cannot be found. Since the numerical values given in these handbooks for the specific heat of indium and the thermal conductivity of indium are identical, it has been suggested that probably the value for the specific heat of indium was misprinted as also the value for the thermal conductivity of indium. One is led to wonder how many technological applications of indium could have been adopted earlier, or for how many heat transfer problems, over a 30-year span, might indium have provided a ready solution, had its thermal conductivity been known to be 3.4 times greater than that listed in major reference works, and higher than that of iron or platinum?

In the 1979 Edition of the Metals Handbook, some of the erroneous values given in the 1961 Edition have been revised, partly by the adoption of CINDAS recommended values. However, some other erroneous old values are still retained

in the 1979 Edition, which gives thermal conductivity values for 62 elements. Of the 62 values given in the 1979 Edition for the 62 elements around room temperature, 7 are still in error by over 20 percent, 5 of the 7 are in error by over 30 percent, 4 of the 5 are in error by over 40 percent, and one of the 4 is in error by 168 percent.

In order to show the comparison of the thermal conductivity values given in the 1961 and the 1979 Editions of the Metals Handbook with CINDAS recommended values, Table 1 lists the thermal conductivity values for 22 selected elements and also the differences in percent between the values given in the Metals Handbook and the values recommended by CINDAS*. It can be observed from Table 1 that even in the latest 1979 Edition there are still many erroneous values given, which is unfortunate. It should be pointed out also that several of these erroneous values retained in the 1979 Edition such as those given for chromium, cobalt, and silicon actually have their earlier origin in the 1948 (Seventh) Edition of the Metals Handbook; that is, the same erroneous values have been repeated in all the 1948, 1961, and 1979 Editions, and no attempt was made to improve these values despite the availability of numerous new experimental data and of recommended reference values. However, what is even more unfortunate is the fact that the inadequacy of general handbooks and reference books as sources of data is not recognized by most users, nor is it acknowledged by editors and publishers.

Among the elements for which the same inaccurate values (as those given in the 1961 Edition) or worse values are given in the latest 1979 Edition of the Metals Handbook, the following elements are notable.

Chromium - The same value, which is believed 29% too low, is given again in the 1979 Edition. However, the author of this section on chromium in the 1979 Metals Handbook did not take this same value from an earlier edition of the Metals Handbook; instead, he took this "new" value from a 1973 5-volume reference work entitled "Comprehensive Inorganic Chemistry." Such a general reference work is certainly not a good source for data on material property, and the author on chromium might not even be aware of the over 20 primary data sources or the sources for recommended reference values for the thermal

* CINDAS' recommended values for the thermal conductivity of the elements are given in most cases for a full range of temperature from near the absolute zero to the melting point of the element or beyond, not just for room temperature as given in Table 1.

Table 1. Comparison of Room-Temperature Thermal Conductivity Values of Selected Elements Given in the Metals Handbook with CINDAS' Recommended Values*

Element	CINDAS (1974)	Metals Handbook (1961)		Metals Handbook (1979)	
	λ (W m ⁻¹ K ⁻¹)	λ (W m ⁻¹ K ⁻¹)	Diff. (%)	λ (W m ⁻¹ K ⁻¹)	Diff. (%)
Antimony	24.4	18.8	-23	25.9	6
Beryllium	201	146	-27	190	-5
Calcium	190 172(200°C)	126	-33	146(200°C)	-15
Carbon (graphite)	5.73 to 1960	24	319 to -99	---	---
Chromium	93.9	67	-29	67	-29
Cobalt	100	69	-31	69.04	-31
Erbium	14.5	9.6	-34	14.5	0
Gadolinium	10.5	8.8	-16	10.5	0
Gallium	40.6	29 to 38	-29 to -6	33.49	-18
Indium	83.7(0°C) 81.8	24	-71	86.6(0°C)	3
Iridium	147	59	-60	147	0
Iron	83.5(0°C) 80.4	75(0°C)	-10	80.4	0
Magnesium	156	154	-1	418	168
Neodymium	16.5(-2.22°C) 16.5	13(-2.22°C)	-21	16.5	0
Plutonium	6.7	8.4	25	6.5	-3
Rhenium	48.1	71.2	48	71.2	48
Rhodium	150	88	-41	150	0
Silicon	149	84	-44	83.680	-44
Tellurium	3.38 (// to c-axis)	5.9	75	3.3 (// to c-axis)	-2
	1.97 (\perp to c-axis)			2.1 (\perp to c-axis)	7
Thorium	54.0	38(100°C)	-30	77	43
	54.3(100°C)				
Titanium	37.9(-240°C)**	11.4(-240°C)		11.4(-240°C)	
	21.9				
Yttrium	17.0(-2.22°C)	14.6(-2.22°C)	-14		
	17.2			17.2	0

*Values are for room temperature unless otherwise specified.

**For polycrystalline titanium having a residual electrical resistivity of $1.90 \times 10^{-8} \Omega \text{ m}$.

conductivity of chromium available in the literature. It is interesting to note that the reference to the source of this value on the thermal conductivity of chromium given in "Comprehensive Inorganic Chemistry" is a 1967 3-volume reference work entitled "Metals Reference Book" (4th Edition), and the reference to the source of this value given in "Metals Reference Book" is a 1943 compilation, which is also the source of the value given in the 1948 Edition of the Metals Handbook. It is therefore no wonder that all these (inaccurate) values are the same.

Cobalt - The same value given for cobalt in all three Editions is believed 31% too low. The only difference is that the value in the latest 1979 Edition has four significant digits ($69.04 \text{ W/m}^2\text{K}$) instead of two. Note that the units given are also wrong. The author gives no reference to any of the property values in the entire section on cobalt prepared by him.

Magnesium - The value (168% too high) given in the 1979 Edition is wrong. The author must have made a mistake either in the conversion of units or some other way. He gives a reference to this value, which is a 1950 survey paper in German entitled "The Relationship Between Thermal and Electrical Conductivities of Aluminum and Magnesium and Their Alloys." However, such a high value for the thermal conductivity of magnesium cannot be found in the original paper.

Rhenium - The same, 48% too high, value is given in the 1979 Edition. The author cites no specific reference for the thermal conductivity value but gives for the entire section on rhenium a general reference, which is a 1975 Russian book entitled "The Study and Use of Rhenium Alloys." There are many data source references in the American literature alone reporting more reliable data, which have all been ignored.

Silicon - Almost the same, 44% too low, value is given in the 1979 Edition, except that the value in this latest Edition has five significant digits (83.680 W/m K) instead of two. The section on silicon is prepared by the same author as the section on chromium, discussed before. He gives no reference to the thermal conductivity value but gives 15 references to other property values. Most of the 15 references given are old books (not research articles), including four published before 1930, six before 1940, and five between 1941 and 1967.

Thorium - While the old value in the 1961 Edition is 30% too low, the new values in the 1979 Edition is 43% too high. The author gives no reference to the thermal conductivity value but gives to the entire section on thorium a general reference, which is a 1975 book authored by himself and his coworkers entitled "Thorium: Preparation and Properties."

Titanium - Titanium is so important a metal in modern technology, yet only the old value given in the 1961 Edition for -400°F (-240°C) is reported in the latest 1979 Edition, and no value is given for room temperature or any other temperature. A thermal conductivity value given for so low a temperature without the accompanying sample characterization is meaningless and useless, and therefore, no comparison can be made with CINDAS' values. In fact, the thermal conductivity of titanium at -240°C can almost be any value depending upon the amount and kind of impurity and the degree of imperfection in the sample.

IV. EXAMPLES OF CRITICALLY EVALUATED, ANALYZED, AND SYNTHESIZED PROPERTY DATA GENERATED BY CINDAS

Using the methods and procedures outlined in Section II, CINDAS has generated recommended values for a large number of properties of numerous materials, examples of which are presented below.

1. Thermal Conductivity of Aluminum

Over 150 sets of experimental data are available for the thermal conductivity of aluminum, part of which are shown, together with recommended values, in Figure 7 in a logarithmic scale and in Figure 8 in a linear scale. The recommended values were generated through evaluation, correlation, and analysis of the available data and through semi-theoretical calculations. At low temperatures the thermal conductivity values for different specimens with small differences in impurity and/or imperfection differ greatly, and a set of recommended values applies only to a particular specimen with a particular amount of impurity and imperfection. The recommended low-temperature values shown in Figure 7 are therefore given as a family of curves, each curve being for a particular specimen with a particular amount of impurity and imperfection as specified by the corresponding value of the residual electrical resistivity, ρ_0 , of the specimen. It can be observed in Figure 7 that each low-temperature thermal conductivity

curve has a maximum, and that the purer the specimen (the smaller the ρ_0), the higher is the maximum conductivity and the lower is the temperature at which the conductivity maximum occurs. Furthermore, the locus of the thermal conductivity maxima is a straight line in a logarithmic plot, such as Figure 7. These low-temperature thermal conductivity values were calculated using reliable methods developed at CINDAS, which have been fully tested. At higher temperatures the thermal conductivity curves converge, and the thermal conductivity of high-purity aluminum can be represented by a single curve as shown in Figure 8. Figure 8 shows also clearly that the recommended values are not at all the averages of the experimental data.

2. Thermal Conductivity of Copper

Figure 9 is an old one produced in 1964 and shows almost all the thermal conductivity data for copper available in 1964 for temperatures above 100 K. It was found at that time that none of the then existing data for high temperatures can represent the thermal conductivity of high-purity copper, and it was predicted that the thermal conductivity values of high-purity copper should be those indicated by the recommended curve shown in Figure 9*. These recommended values were published in NSRDS-NBS 8. Three years later, the predicted values were confirmed by accurate measurements on high-purity copper at the National Research Council of Canada; the differences between the NRC experimental data and the CINDAS predicted values are mostly smaller than one percent.

3. Thermal Conductivity of Nickel + Copper Alloys

The available experimental data on the thermal conductivity of nickel + copper alloys are shown in Figure 10. These fragmentary and often conflicting data were critically evaluated and analyzed. In the meantime, we developed reliable methods for the calculation of electronic and lattice thermal conductivities of alloys. The electronic thermal conductivity of an alloy was calculated from the electrical resistivity and thermoelectric power of the alloy and the electrical resistivity and thermal conductivity of the pure constituent elements. The lattice thermal conductivity was calculated semi-theoretically, based upon the Klemens-Callaway theory. The reliability of these methods was fully tested with selected key sets of accurate experimental data on alloys in various binary

* The recommended curve for the thermal conductivity of copper has subsequently been slightly modified.

alloy systems. From the critically evaluated experimental data and the values calculated from the CINDAS developed methods, recommended thermal conductivity values for the alloys were generated, as presented in Figure 11, which cover a full range of temperature and composition. Figure 11 shows also the Curie temperature of each alloy as the point at which the slope of the curve changes abruptly.

4. Thermal Conductivity of Aluminum + Copper Alloys

As the reliability of methods for the calculation of thermal conductivity of alloys is affirmed, thermal conductivity values can be generated even if the available experimental data are very limited and fragmentary. The thermal conductivity of aluminum + copper alloys is one of such cases. The merit of data synthesis can best be appreciated by comparing the available few experimental data shown in Figure 12 and the full-range recommended values presented in Figure 13.

5. Electrical Resistivity of Copper

There are over 300 sets of experimental data available for the electrical resistivity of copper, part of which are shown, together with the recommended values, in Figures 14 and 15. The available data were critically evaluated and analyzed. The analysis of electrical resistivity data for an element such as copper was mainly on the intrinsic resistivity, the recommended values for which were generated. At low temperatures the electrical resistivity values for different specimens with small differences in impurity and/or imperfection differ greatly due to the differences in their residual resistivity, as shown in Figure 14. Hence, the recommended values shown in the figure at temperature below 55 K are applicable only to a particular specimen with a residual electrical resistivity of $0.00200 \times 10^{-8} \Omega \text{ m}$. A family of low-temperature curves, each for a particular specimen with a particular residual electrical resistivity, can be generated by adding the various residual resistivity values of the specimens to the recommended values of the intrinsic resistivity.

6. Electrical Resistivity of Nickel + Copper Alloys

The available experimental data on the electrical resistivity of nickel + copper alloys are shown in Figure 16. These data were likewise critically evaluated, analyzed, and synthesized. In analyzing the electrical resistivity data for alloys, the intrinsic resistivity and residual resistivity were analyzed separately and then were combined with the amount of the deviation from the Matthiessen's rule to obtain the total electrical resistivity. The resulting recommended values are presented in Figure 17 which cover a full range of temperature and composition. The Curie temperature of each alloy is also shown in Figure 17, clearly as the point at which the slope of the curve changes abruptly.

7. Thermoelectric Power of Nickel + Copper Alloys

The available experimental data on the thermoelectric power of nickel + copper alloys are shown in Figure 18. From these limited fragmentary data, recommended values were generated to cover a full range of temperature and composition as shown in Figure 19. On comparison of Figures 19, 17, and 11, it can be observed that the magnetic transition (around the Curie temperature) has a more remarkable effect on the thermoelectric power of these alloys than on the other properties.

8. Thermal Linear Expansion of Iron, Plutonium, and Uranium

The available experimental data on the thermal linear expansion of iron, plutonium, and uranium are shown, respectively, in Figures 20, 21, and 22 together with the recommended values, which were generated through evaluation and analysis of the available data. Figure 20 shows also the experimental data and recommended values for the coefficient of thermal linear expansion of iron. It is important to note the different ordinate scales for different curves in Figures 21 and 22.

9. Thermal Linear Expansion of Nickel Steels

Figure 23 shows the available experimental data on the thermal linear expansion of nickel steels and the provisional values generated through evaluation and analysis of the available data. Shown also are the available experimental data and provisional values for the coefficient of thermal linear expansion.

10. Normal Spectral Reflectance of Stainless Steels

The available experimental data on the normal spectral reflectance of stainless steels are presented in Figure 24, which shows that this property can be almost any value, from near zero to near one (the upper limit). These data were critically evaluated and analyzed, and the resulting analyzed data are shown in Figure 25. The systematic variation of this property with the surface condition of the material is clearly shown in this analyzed graph. It shows that the reflectance of the most smooth surface is the highest, decreases with increasing surface roughness, and further decreases and becomes undulatory when the surface is oxidized; the latter is due to the absorption band of the resulting oxides. By comparing Figures 24 and 25, one would be further convinced that data analysis is a power tool to bring order out of very chaotic experimental observations.

11. Normal Spectral Emittance of Inconel

Figure 26 shows the available experimental data on the normal spectral emittance of Inconel, which likewise cover the full range of possible values from near zero to near one. The analyzed data are presented in Figure 27, which shows that, contrary to the reflectance, the emittance of the most smooth surface is the lowest, increases with increasing surface roughness, and further increases and becomes undulatory when the surface is oxidized; the latter is likewise due to the absorption band of the resulting oxides.

12. Refractive Index of Alkali Halides and Its Temperature and Wavelength Derivatives

The refractive index (n) of most alkali halides has received few measurements. Of the twenty alkali halides, sufficient data are available for only six. On a number of them, measurement has been made only at one single wavelength. Sodium chloride is one of the few halides whose refractive index has been extensively measured, and the available experimental data for sodium chloride in the transparent wavelength region are shown in Figure 28. In data analysis and synthesis for the few halides with sufficient data such as sodium chloride, it was found, fortunately, that the dispersion formula of the Sellmeier type fits the data for all of them well. The good fit of the theoretical Sellmeier equation to the experimental data for sodium chloride can be seen in Figure 28 by comparing the

recommended values with the experimental data. Consequently, full-range refractive index values for all the alkali halides (including those with only one single experimental data point) could be generated from the Sellmeier equation by using as input one or a few evaluated reliable experimental data on the refractive index and some auxiliary known data on the static and high-frequency dielectric constants and the spectral positions of absorption bands. Figure 29 shows the two experimental data points (the lower one of which is far off) available for the refractive index of lithium chloride and CINDAS recommended and provisional values which cover a full range of wavelength. The resulting full-range values for the refractive index of all the twenty alkali halides are shown in Figure 30.

Regarding the temperature coefficient of the refractive index (dn/dT) of alkali halides, the available information is even more scanty. Only five of the twenty alkali halides have received reasonable attention, and no measurement has ever been made on thirteen of them. Although there are a number of physical properties of alkali halides such as static and high-frequency dielectric constants, wavelengths of absorption bands, and oscillator strengths available at our disposal in the formulation of the equation for the temperature derivative of refractive index, the prediction for the unmeasured material is hampered by certain unknown parameters in the equation. However, these difficulties were fortunately overcome by the discovery of two empirical relations based on the existing data for the five measured alkali halides (LiF, NaF, NaCl, KCl, CsI). The first is the relation that the derivative of the logarithm of the effective wavelength of ultraviolet absorption band (λ_u) with respect to temperature is related to the atomic number of the alkali ion by a power law, as shown in Figure 31, where the value for the four rubidium halides and for other unmeasured materials can easily be predicted. The second is a linear relationship between the ratio of the effective thermal linear expansion (α') to the true thermal linear expansion (α) and the atomic number of the alkali ion, as shown in Figure 32, where the effective thermal linear expansion was obtained by assuming that the temperature coefficient of refractive index is totally due to density change. By using these two empirical relations, the temperature derivative of refractive index of all the alkali halides were generated and the results agree remarkably well with the existing experimental data. The agreement of the calculated values with the experimental data for dn/dT of sodium chloride is shown in Figure 33, while the resulting values for dn/dT for all the twenty alkali halides are presented in Figure 34.

From the Sellmeier equation for the refractive index, the wavelength derivative of refractive index ($dn/d\lambda$) for all the twenty alkali halides could be generated and the results are presented in Figure 35.

13. Refractive Index of Silicon and Its Temperature Derivative

Figures 36 and 37 show all the available experimental data on the refractive index of silicon for the wavelength and temperature dependences, respectively. From these fragmentary and often conflicting data, recommended values were generated as presented in Figure 38 which cover a full range and are as a function of both wavelength and temperature. Such a complete spectrum of values on the refractive index of silicon is for the first time ever available. Similarly, Figure 39 presents the recommended values for the temperature derivative of the refractive index of silicon as a function of both wavelength and temperature.

14. Absorption Coefficient of Calcium Fluoride

The available experimental data on the absorption coefficient of calcium fluoride are shown in Figure 40, with details in the multiphonon region and in the Urbach tail region enlarged in Figures 41 and 42. In the multiphonon region, the discrepancies in the experimental data are mainly due to extrinsic contributions such as by chemical impurities, crystal defects, and surface contamination. The available data indicate that the intrinsic absorption coefficient may be expressed as an exponential function of frequency. Through critical evaluation and careful analysis of the available data, we have not only verified the exponential dependence of the absorption coefficient on the wave frequency, but also successfully introduced the temperature as an additional functional variable, resulting in an equation expressing the absorption coefficient as an exponential function of both frequency and temperature. The recommended values for the absorption coefficient of calcium fluoride are presented in Figures 43 and 44, in which the "crossover point" is also shown.

V. CONCLUSIONS

The above presentation has illustrated CINDAS' general methodology of critical evaluation, correlation, analysis, and synthesis of experimental physical property data and of generation of recommended reference values. It has shown how the fragmentary and conflicting experimental data recorded in the scientific and technical literature can be thoroughly evaluated, analyzed, and synthesized to generate a full field of information hitherto unavailable.

It should be apparent from this presentation that data evaluation, analysis, and synthesis is a very powerful tool which not only can clean up a body of conflicting and chaotic experimental data, but also can create new knowledge, which in itself is a major contribution to science and technology. Thus, TEPIAC/CINDAS can provide to the user not only just any (or all) available data and information (which is usually the limit that an ordinary information center can do), but also evaluated correct data and information, and furthermore, in many cases TEPIAC/CINDAS can provide predicted data and information to the user even when the required data and information are completely lacking and nonexistent.

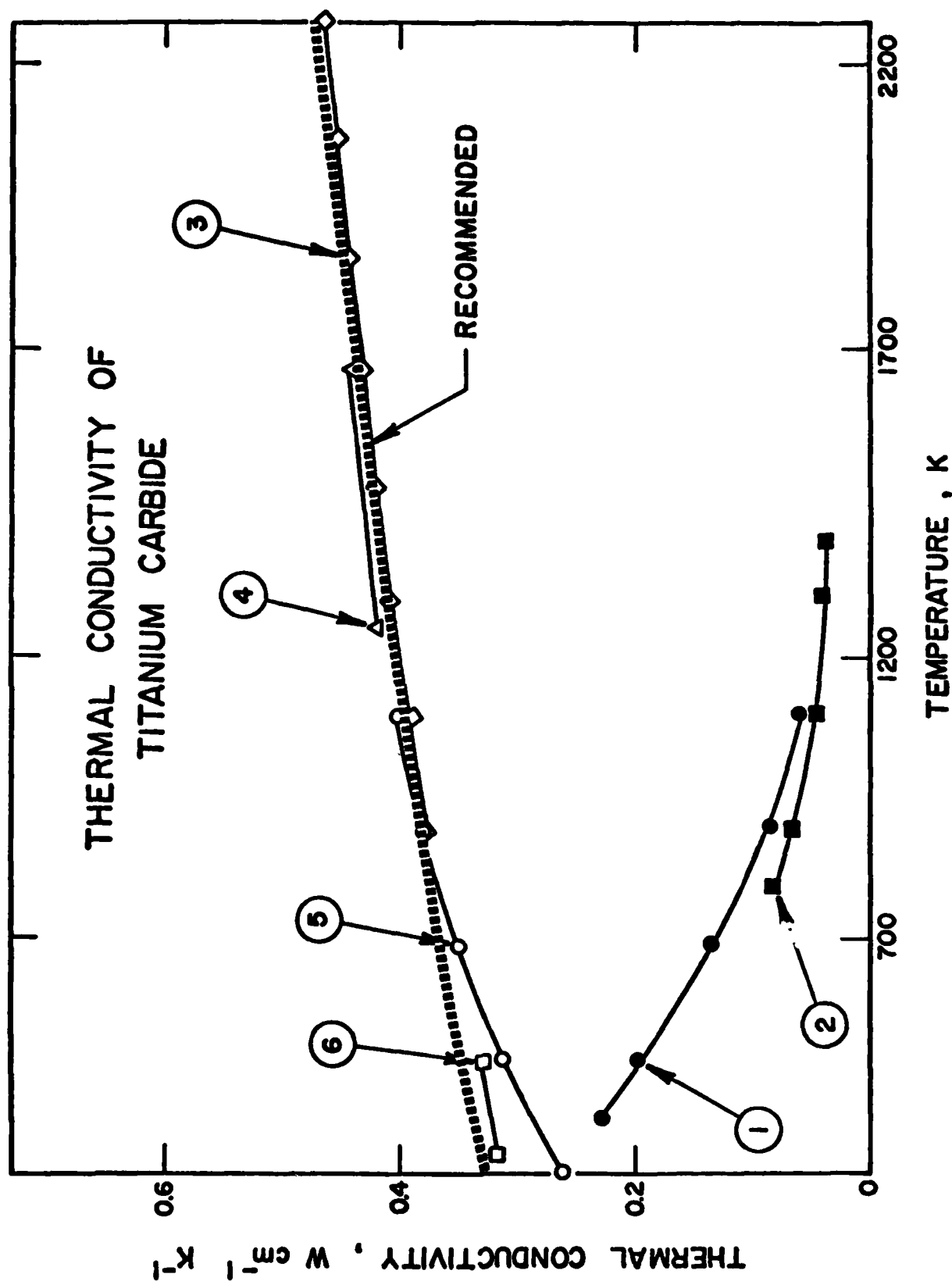


Figure 1. Experimental data and recommended values for the thermal conductivity of titanium carbide. This shows that the lower experimental data are utterly erroneous, being about five times too low at 800 K and ten times too low at 1350 K.

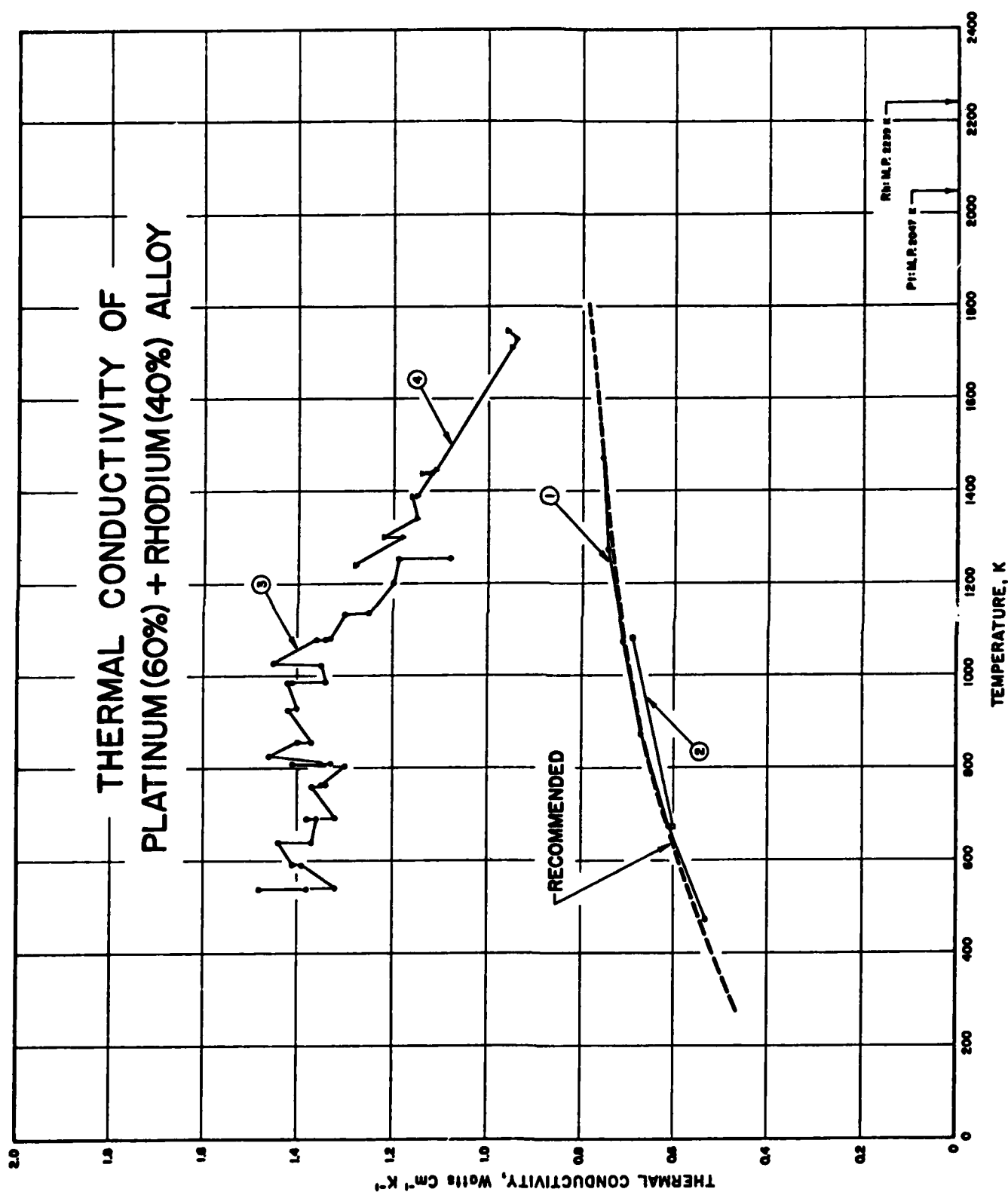


Figure 2. Experimental data and recommended values for the thermal conductivity of platinum (60%) + rhodium (40%) alloy. This shows that the higher experimental data are utterly erroneous, being about 140% too high at 550 K.

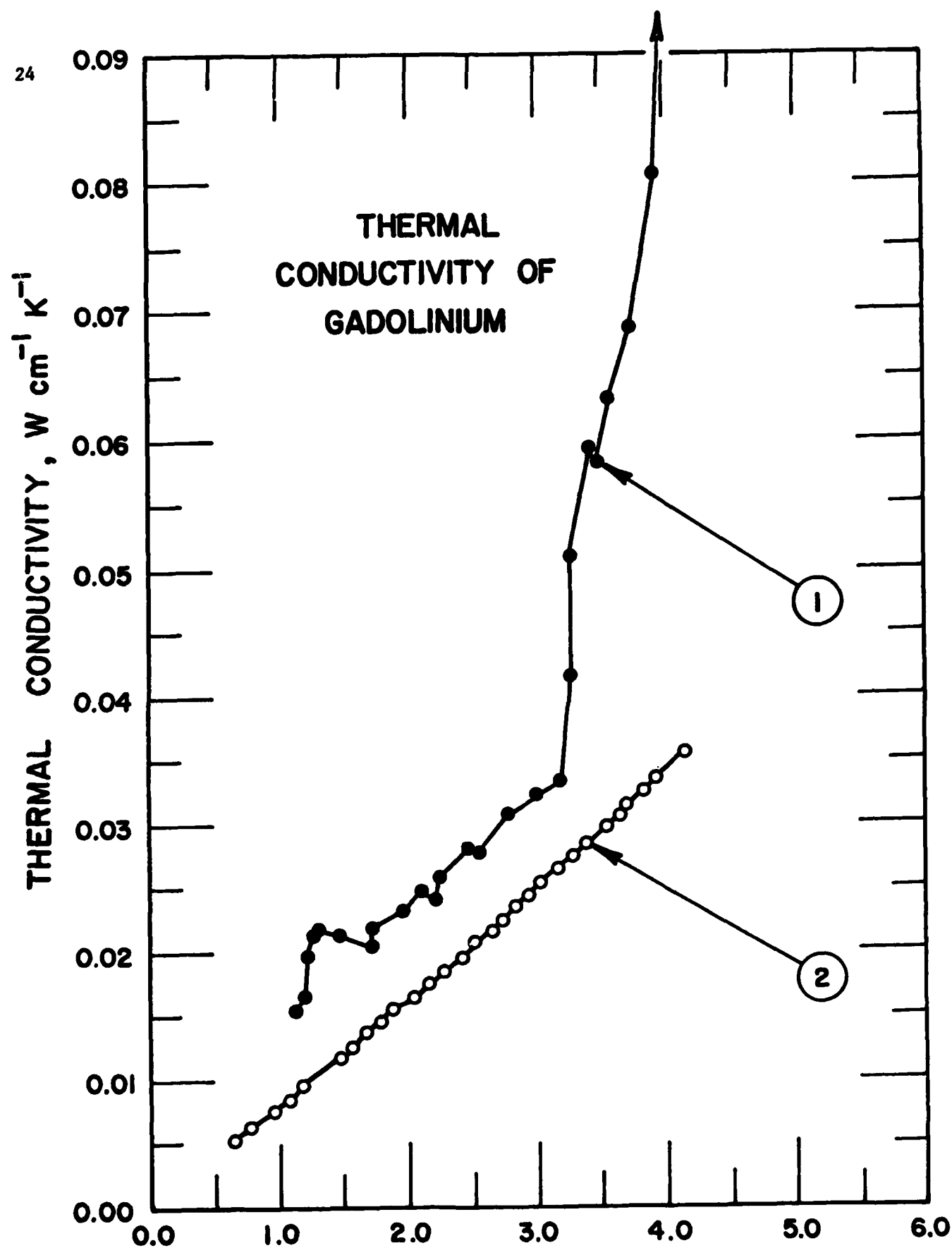


Figure 3. Thermal conductivity of gadolinium. These two sets of experimental data, though widely apart, are for the same one piece of specimen and from the same laboratory.

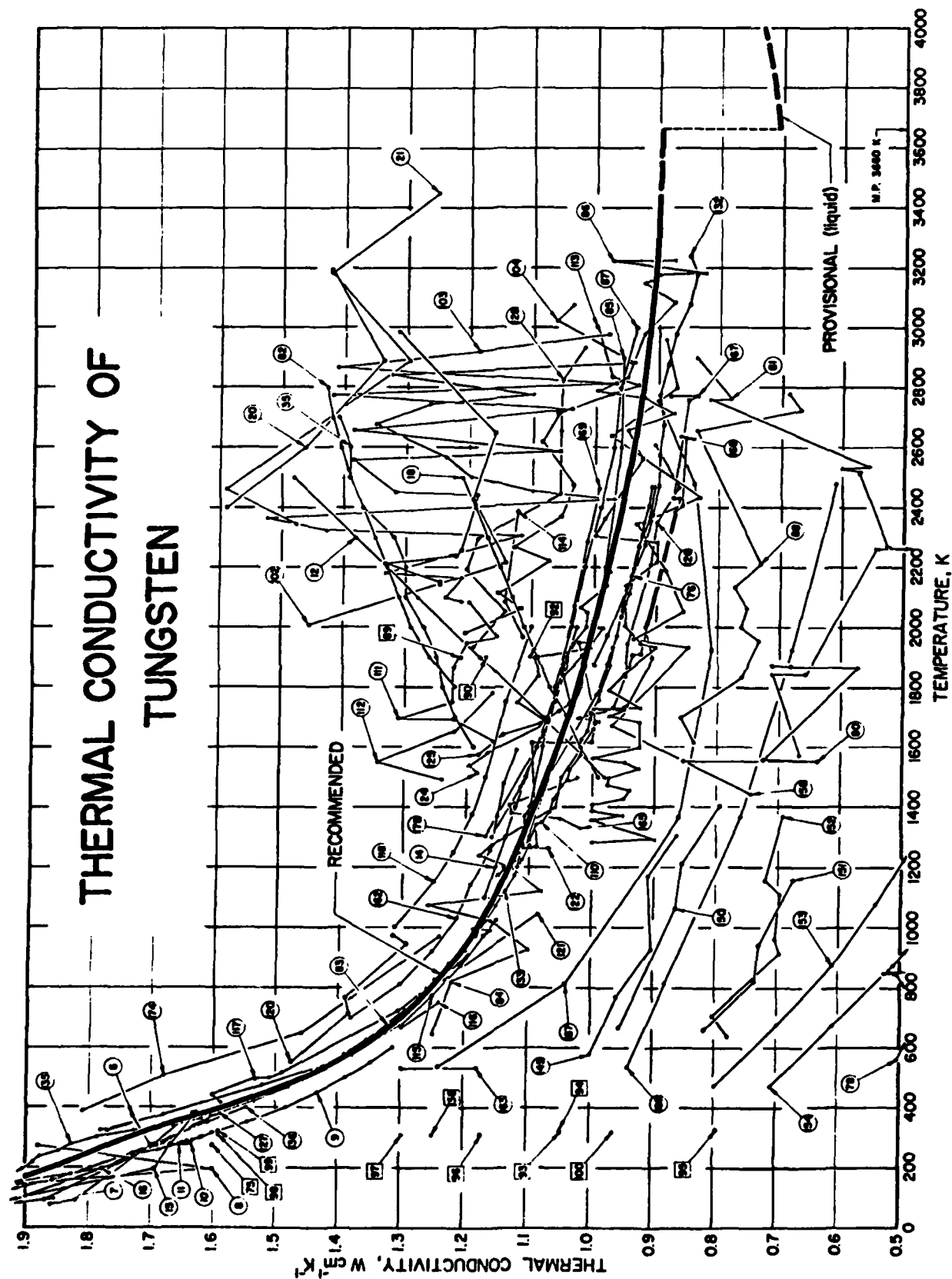


Figure 4. Experimental data and recommended values for the thermal conductivity of tungsten. This shows that most of the experimental data are erroneous, conflicting, and widely diverging.

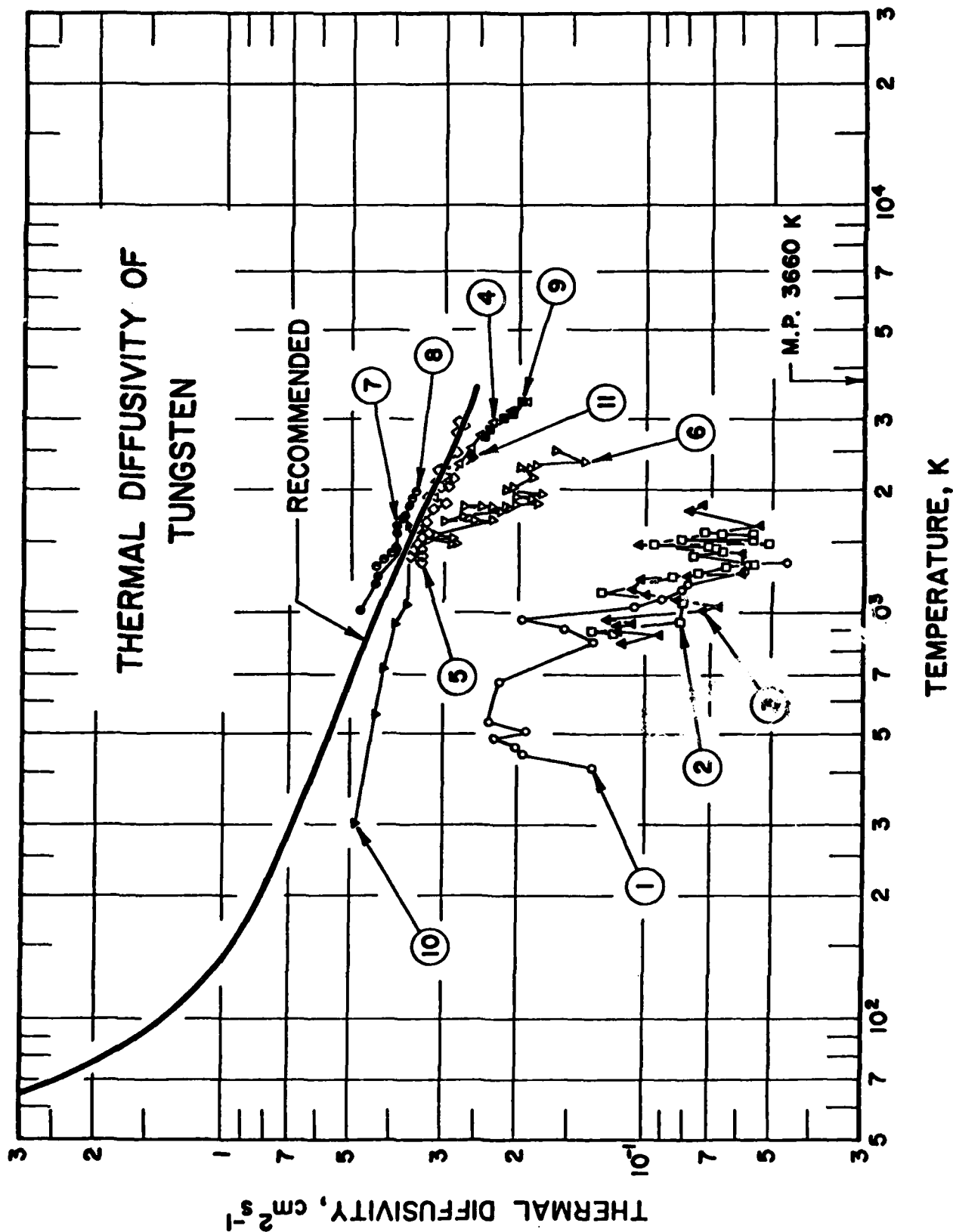


Figure 5. Experimental data and recommended values for the thermal diffusivity of tungsten. This shows that the lower experimental data are utterly erroneous, being about five times too low.

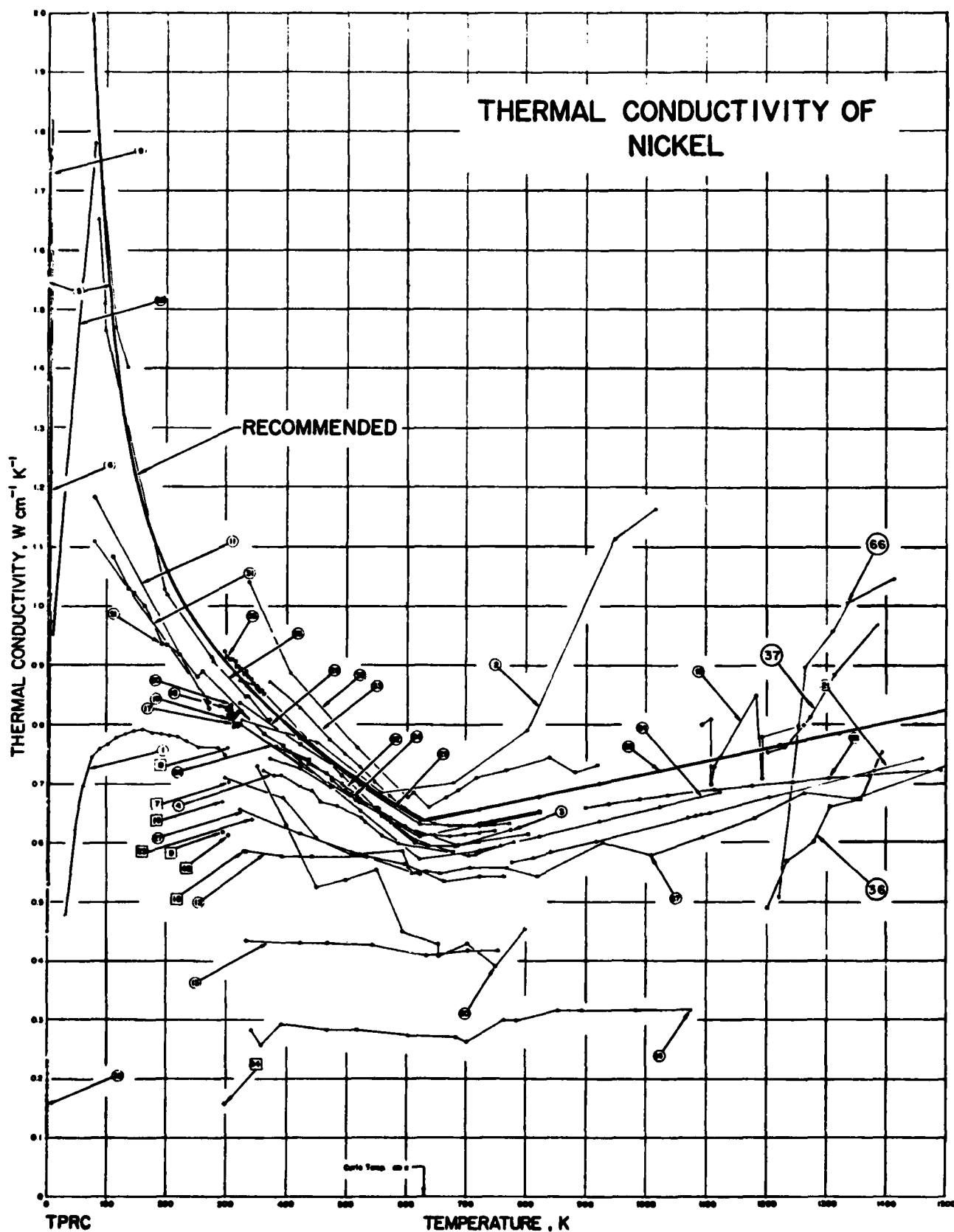


Figure 6. Experimental data and recommended values for the thermal conductivity of nickel.

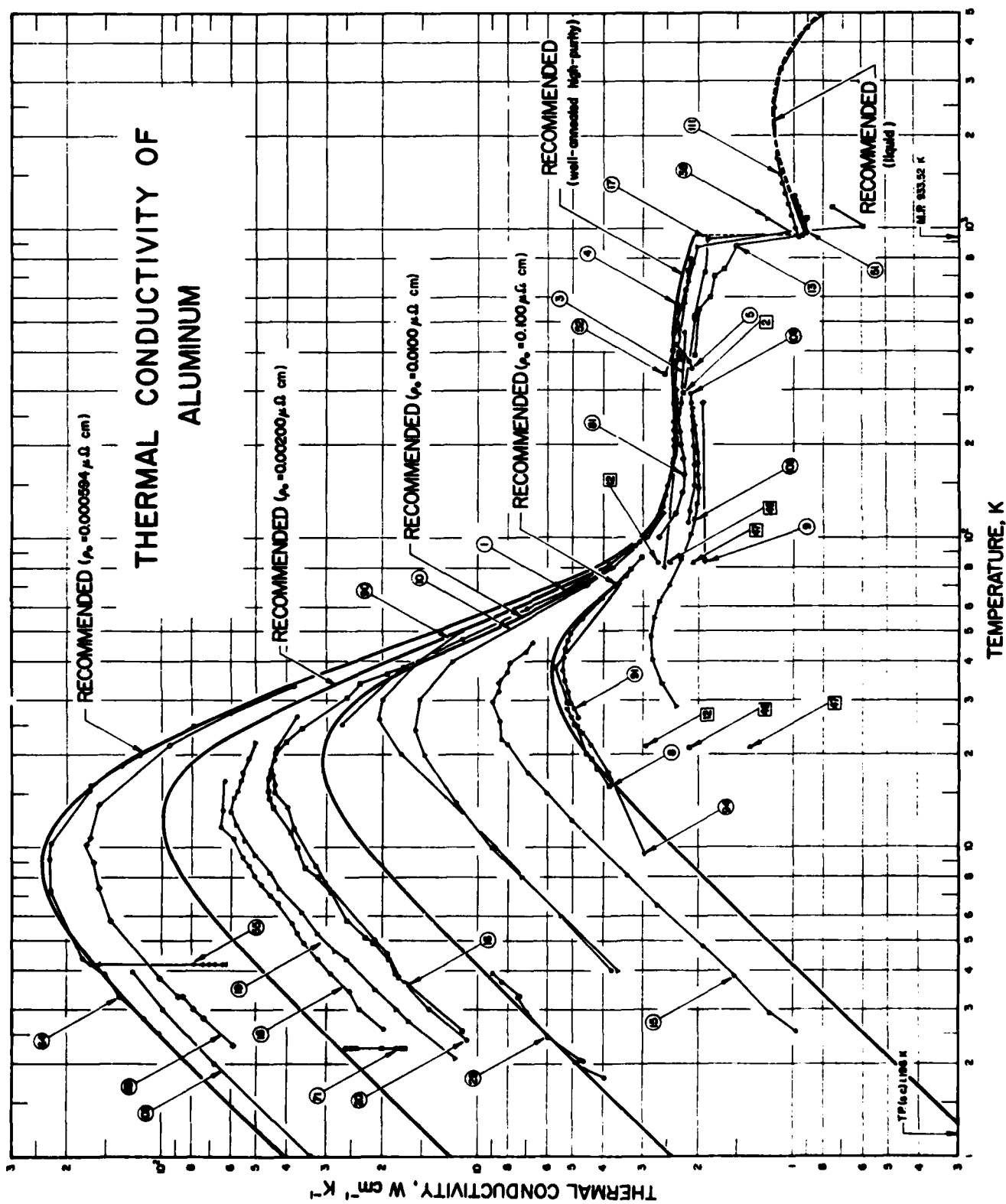


Figure 7. Experimental data and recommended values for the thermal conductivity of aluminum (logarithmic scale).

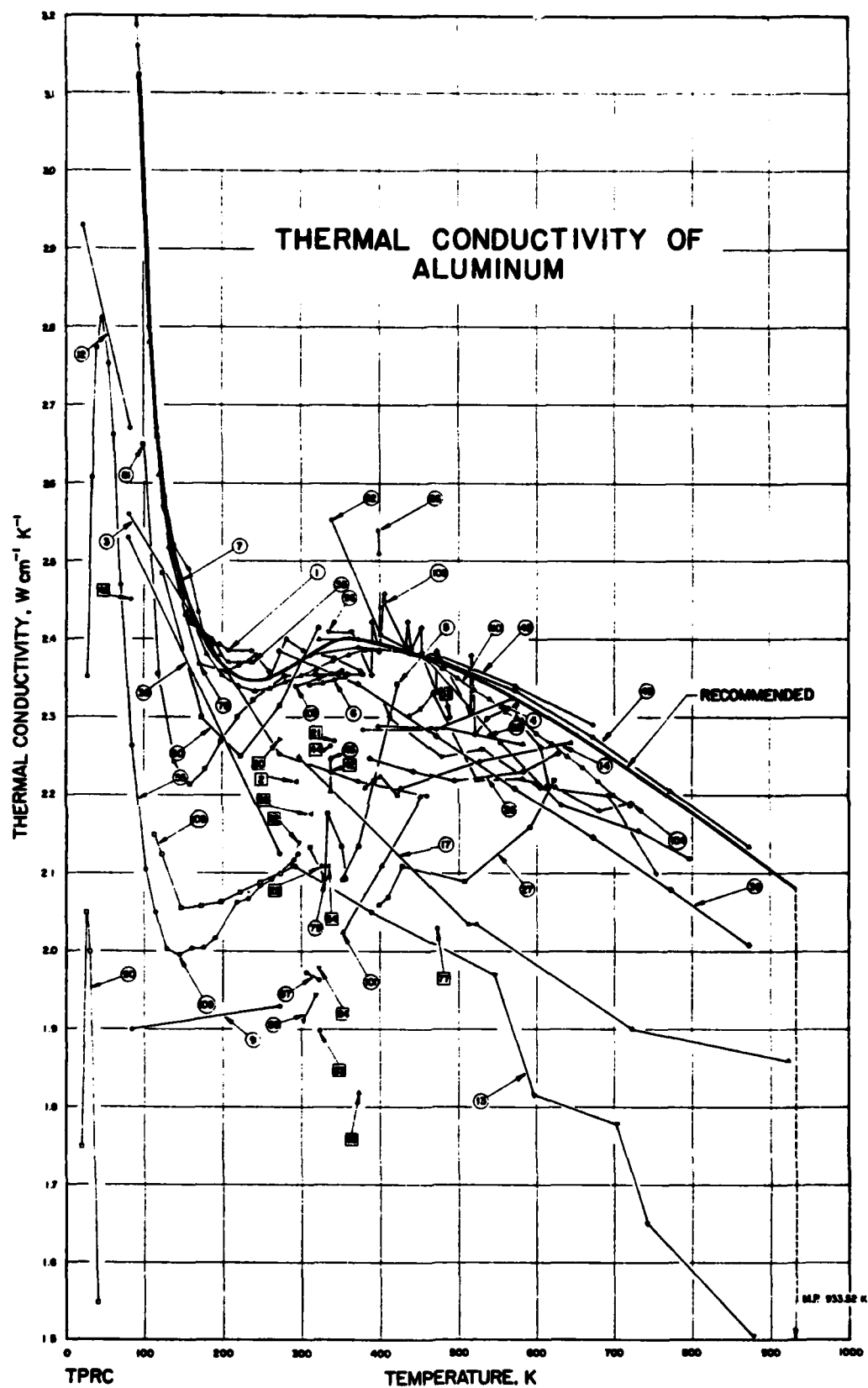


Figure 8. Experimental data and recommended values for the thermal conductivity of aluminum (linear scale).

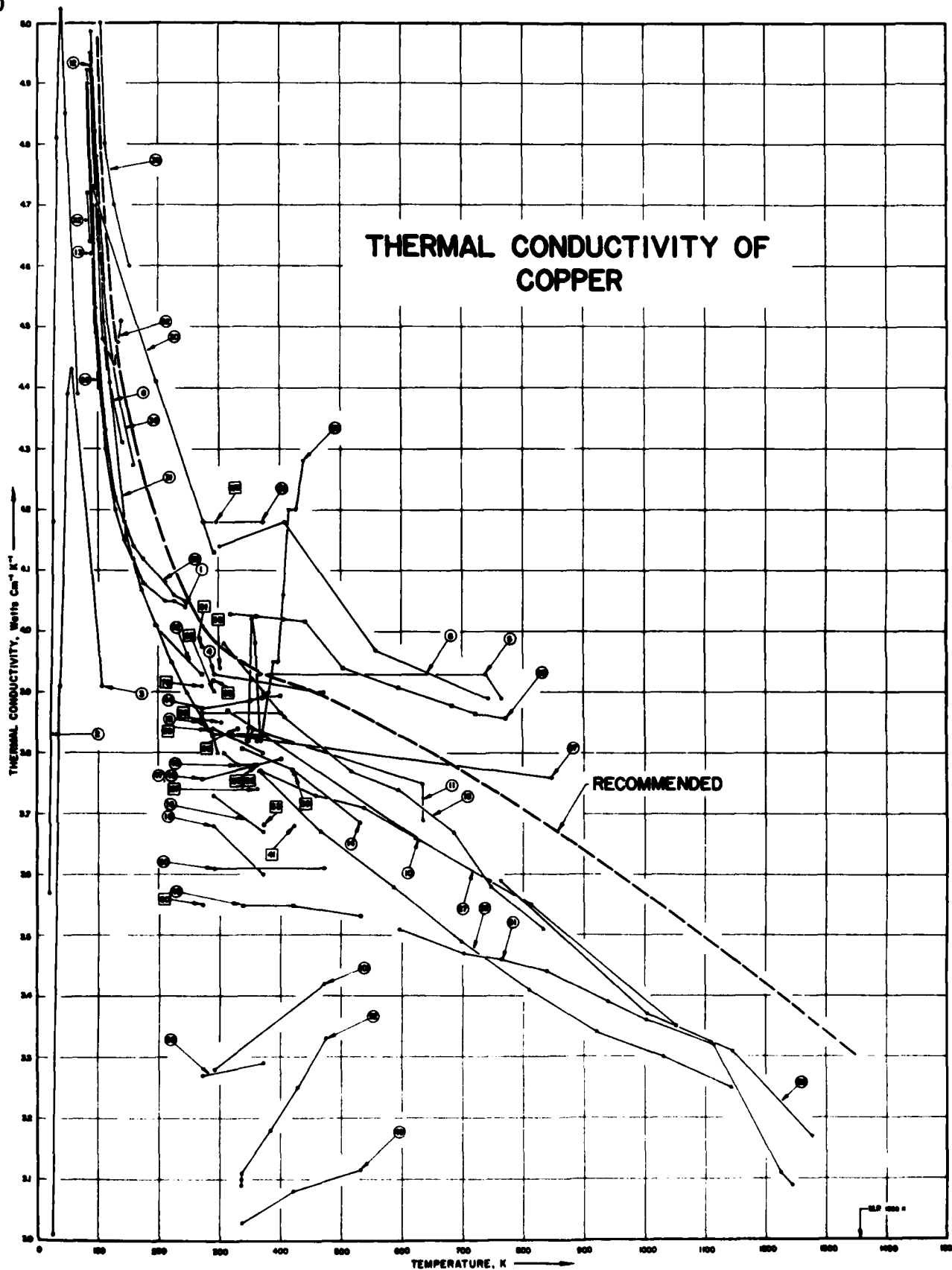


Figure 9. Experimental data and recommended values for the thermal conductivity of copper (as of 1964).

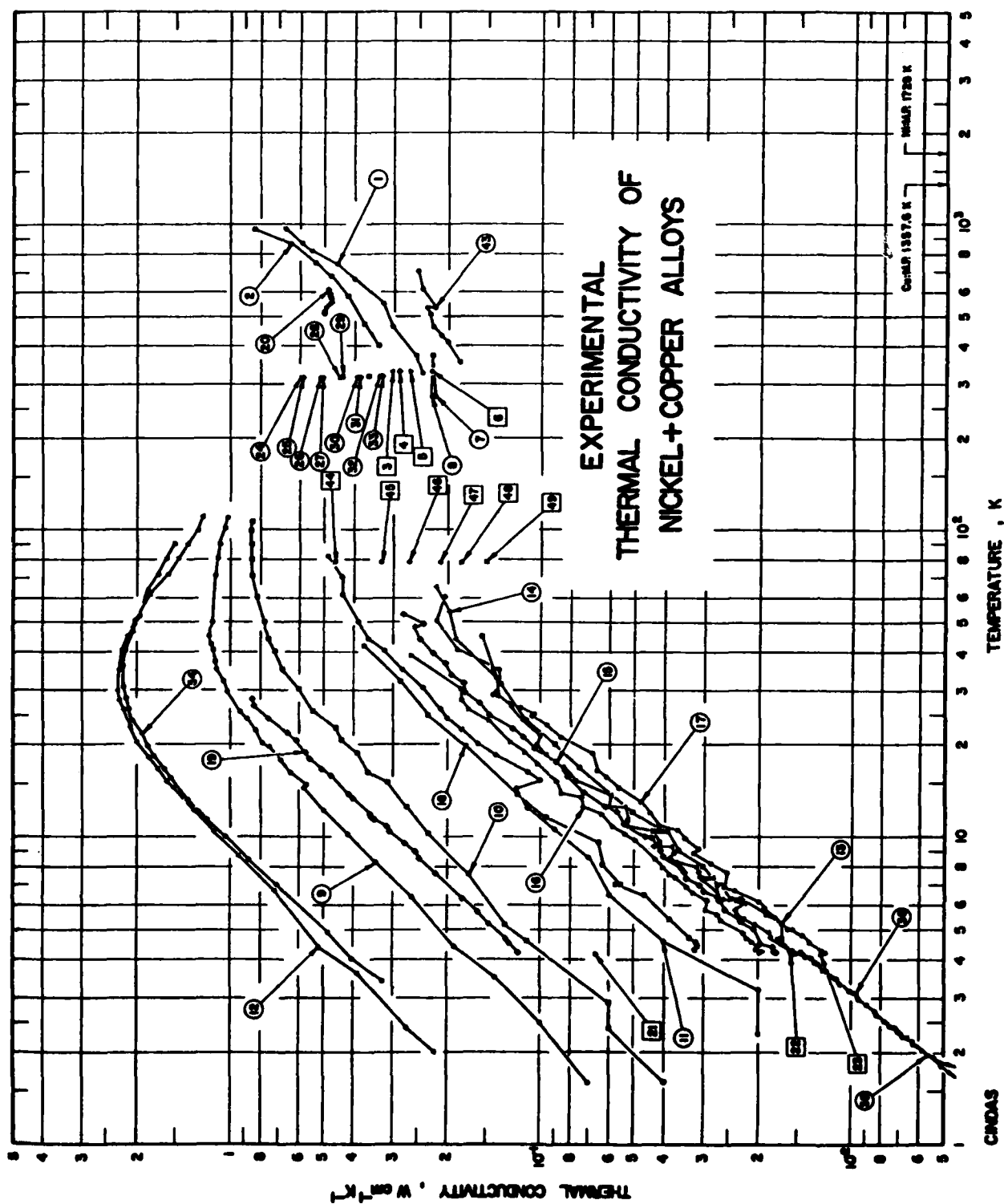


Figure 10. Experimental data on the thermal conductivity of nickel + copper alloys.

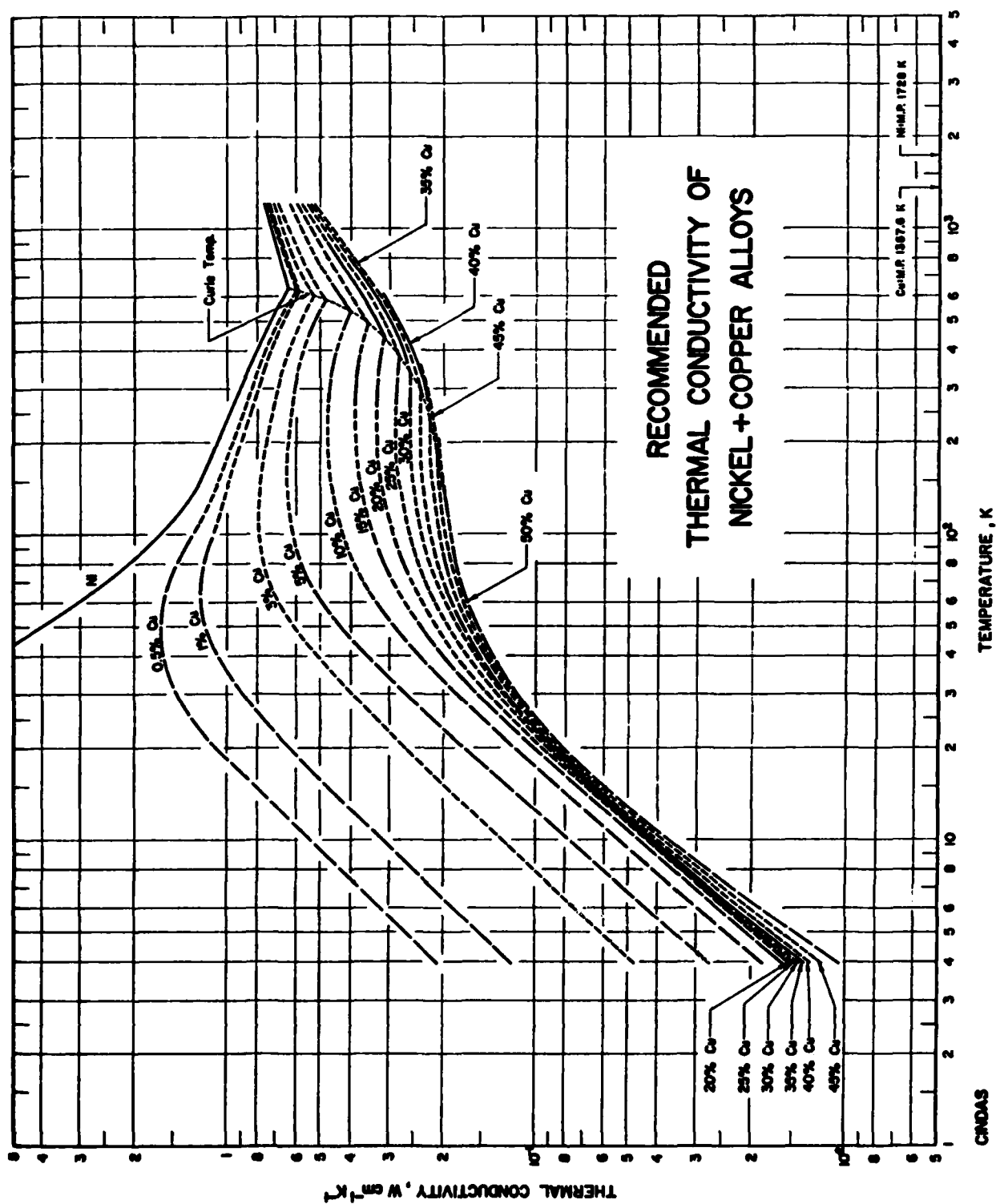


Figure 11. Recommended values for the thermal conductivity of nickel + copper alloys. These recommended values were generated through data evaluation, analysis, synthesis, and semi-theoretical calculations based on the limited experimental raw data shown in Figure 10 and on the available data on the electrical resistivity.

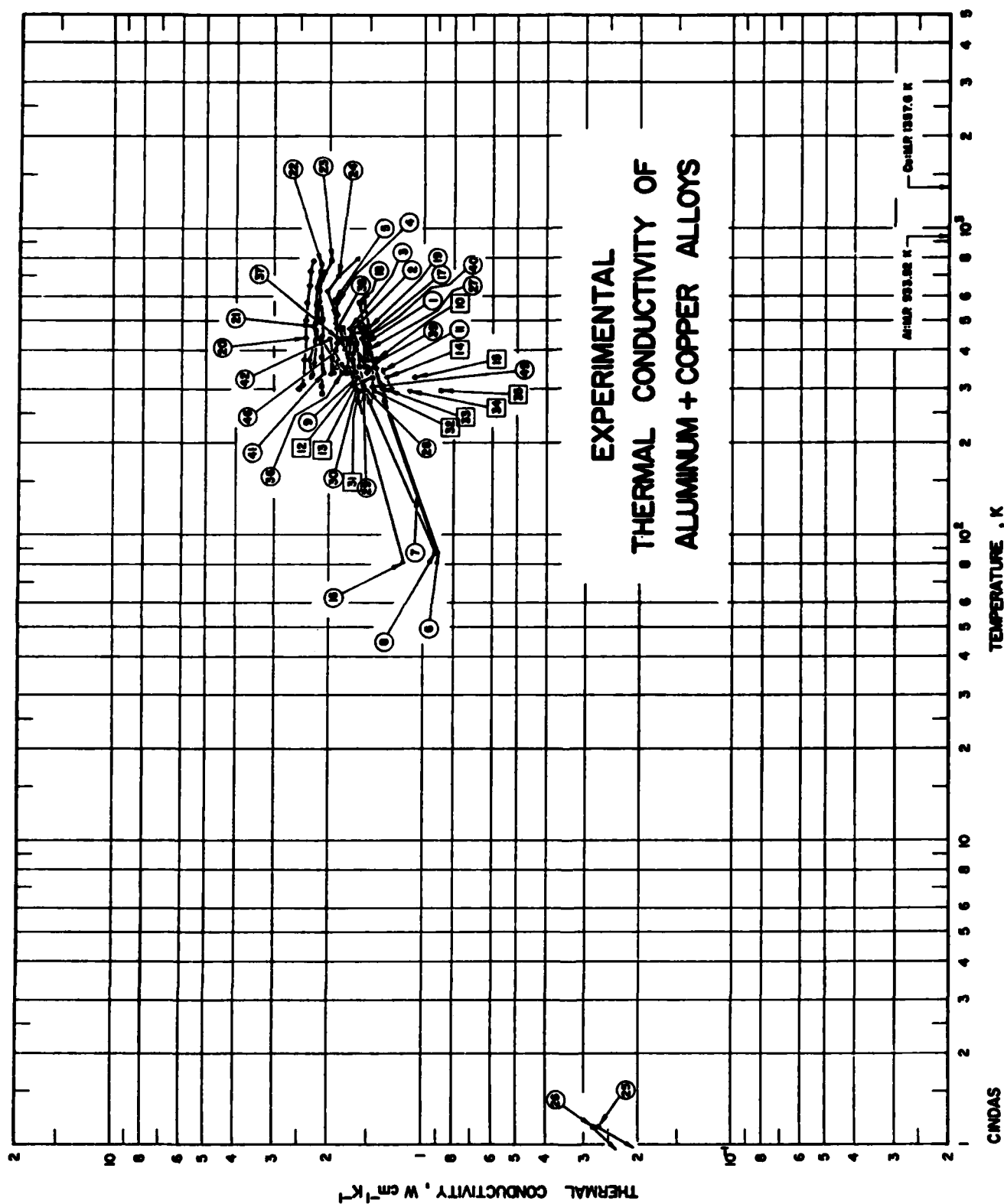


Figure 12. Experimental data on the thermal conductivity of aluminum + copper alloys. These experimental data are very limited, fragmentary, and often conflicting.

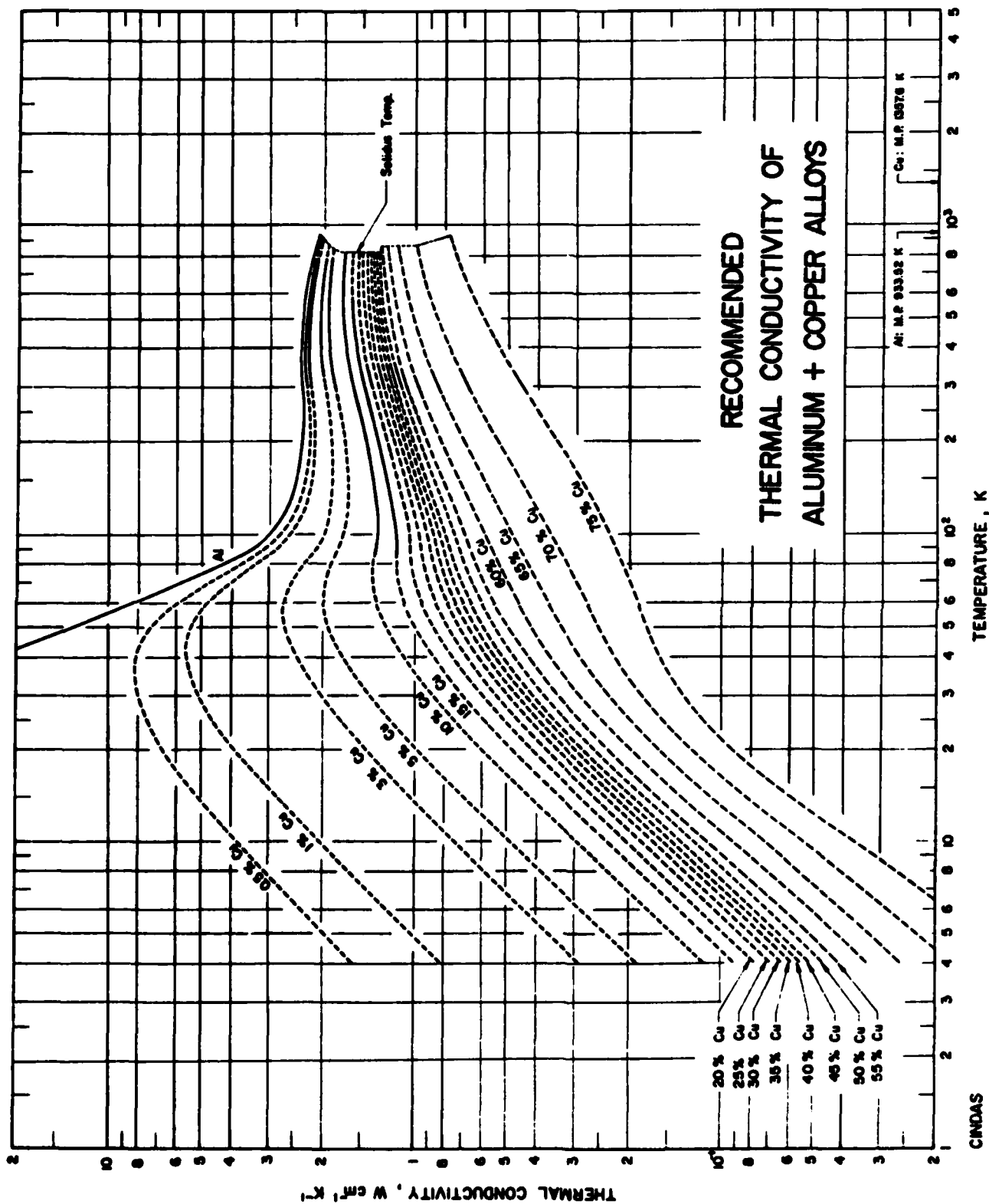


Figure 13. Recommended values for the thermal conductivity of aluminum + copper alloys. These recommended values were generated through data evaluation, analysis, synthesis, and semi-theoretical calculations based on the very limited experimental raw data shown in Figure 12 and on the available data on the electrical resistivity.

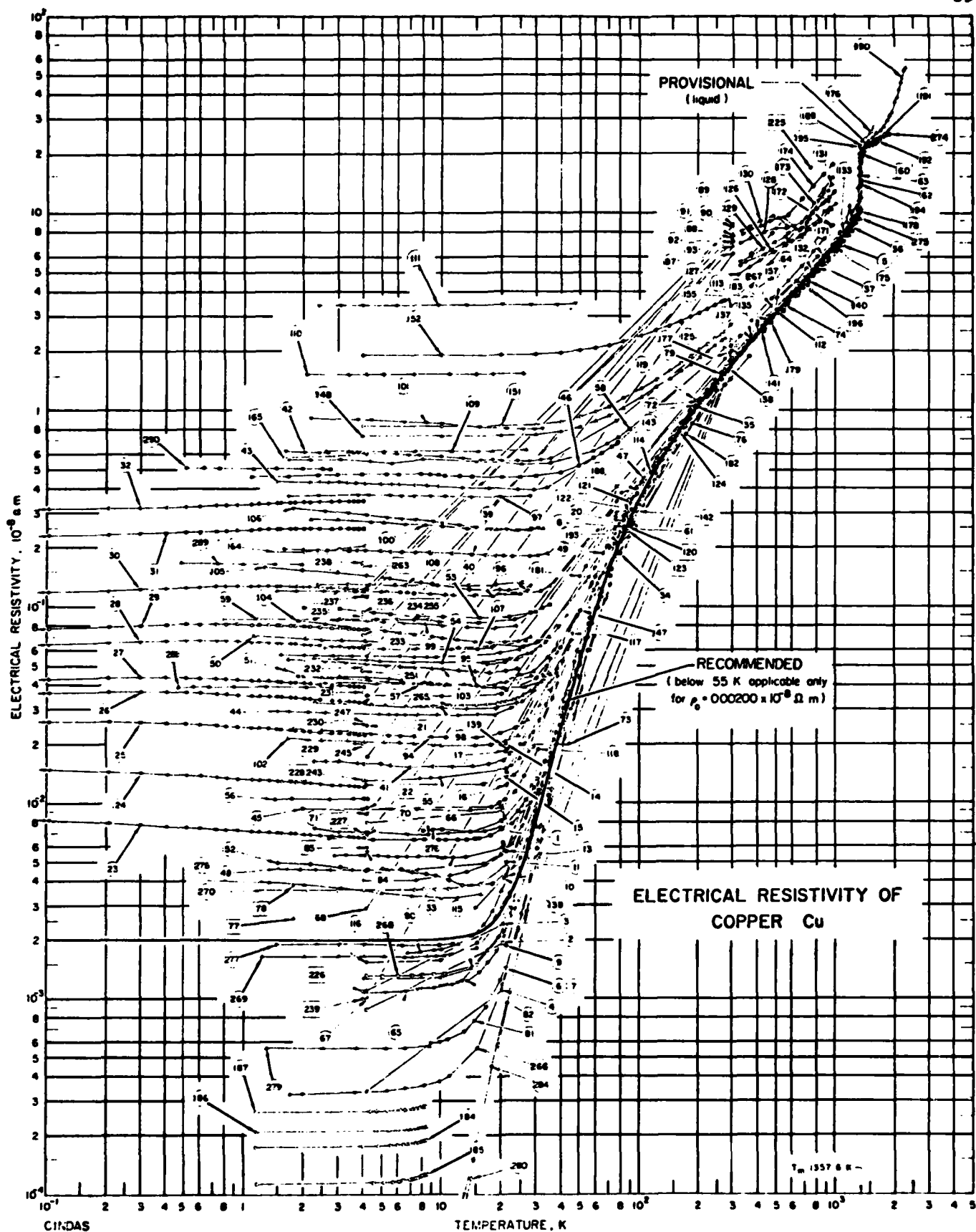


Figure 14. Experimental data and recommended values for the electrical resistivity of copper (logarithmic scale).

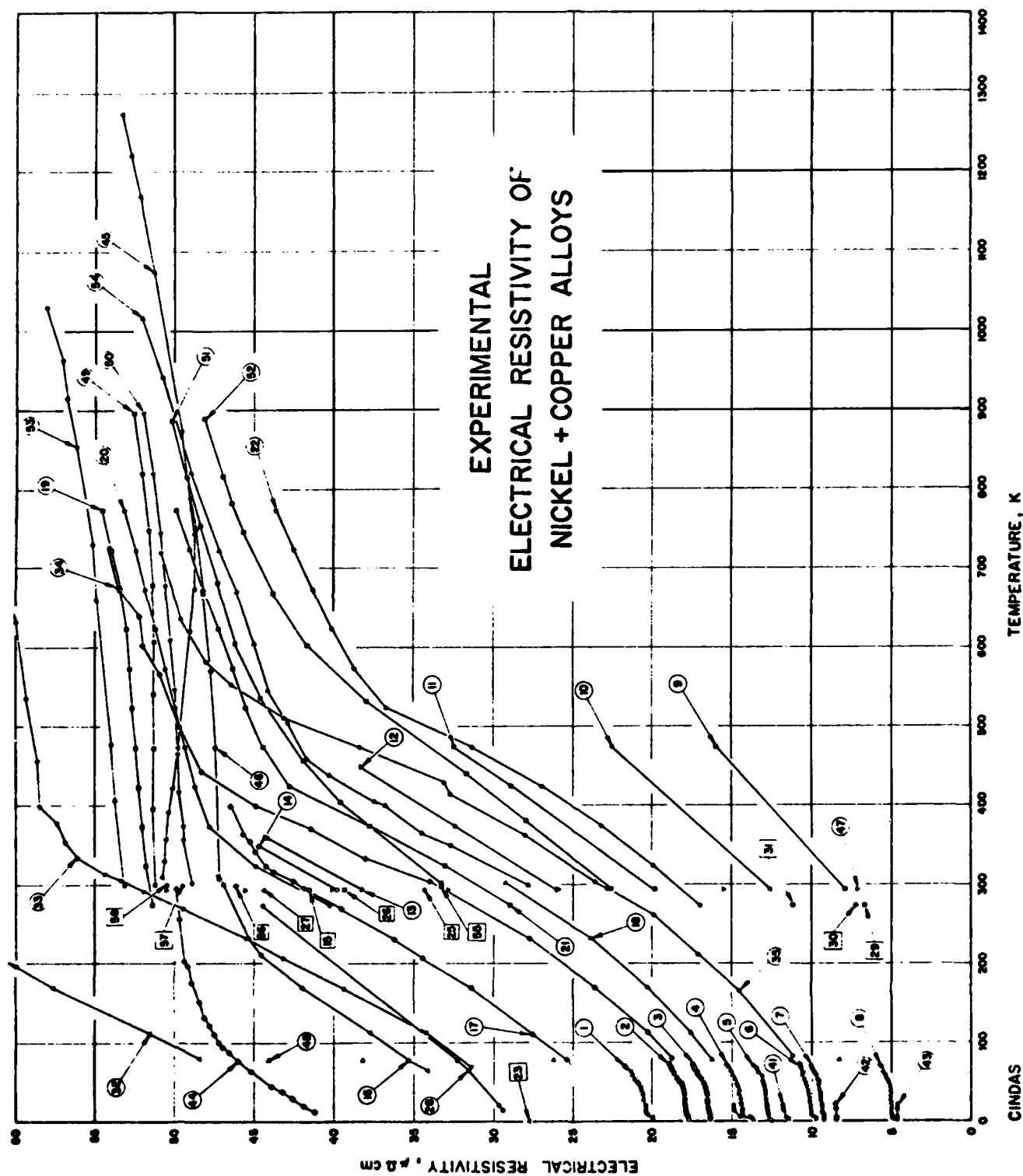


Figure 16. Experimental data on the electrical resistivity of nickel + copper alloys.

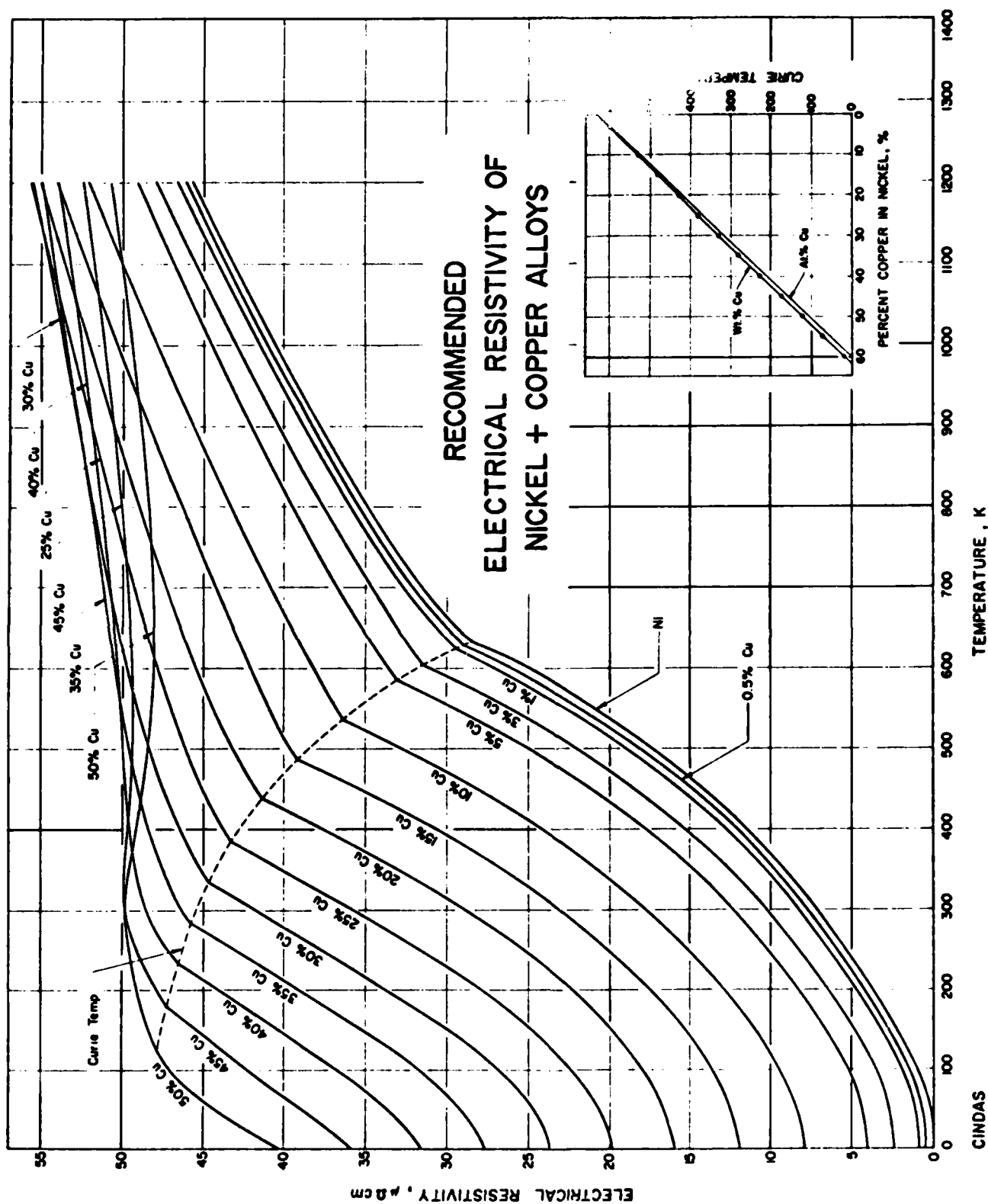


Figure 17. Recommended values for the electrical resistivity of nickel + copper alloys.

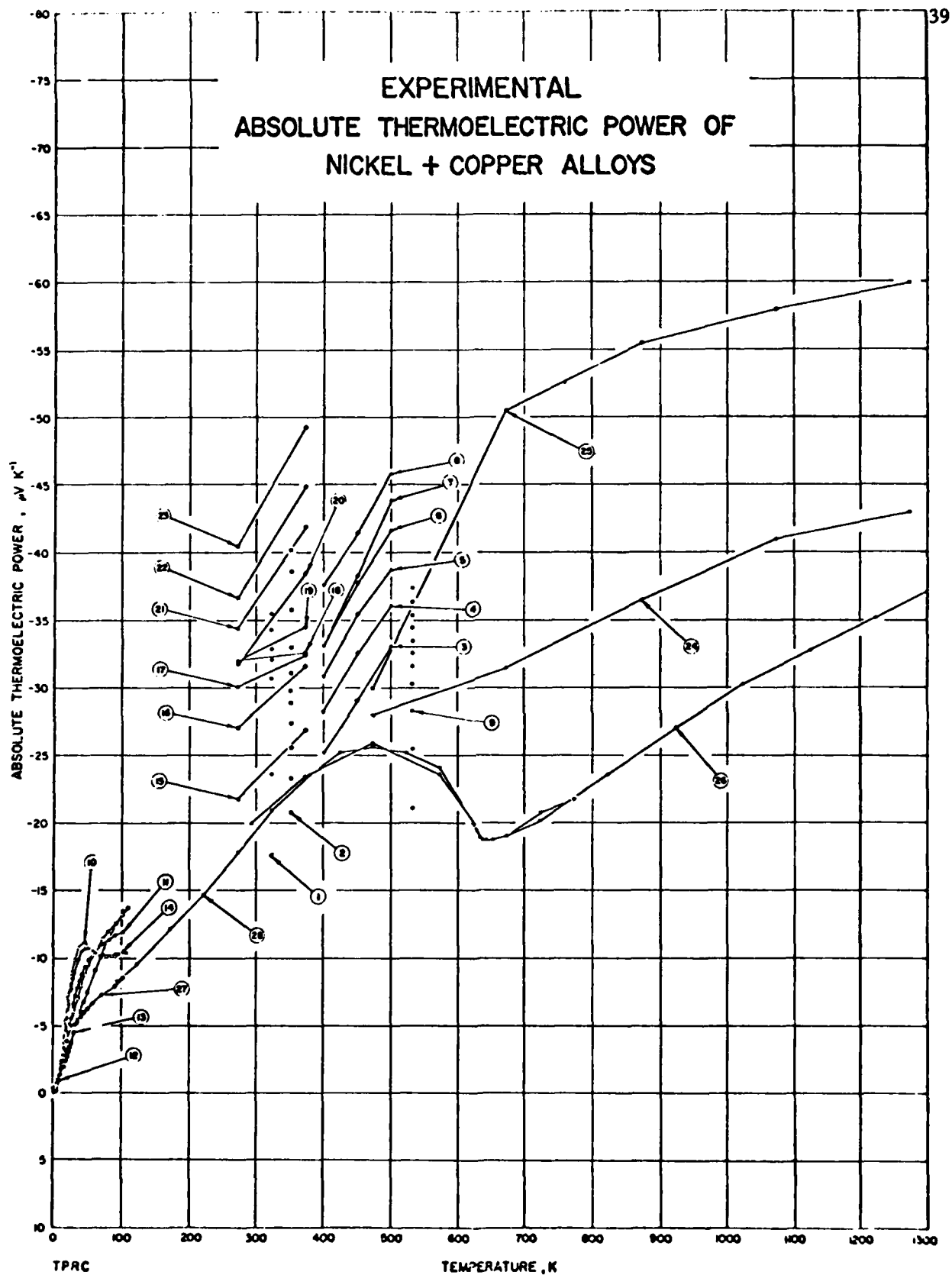


Figure 18. Experimental data on the absolute thermoelectric power of nickel + copper alloys. These experimental raw data are very limited, fragmentary, and conflicting.

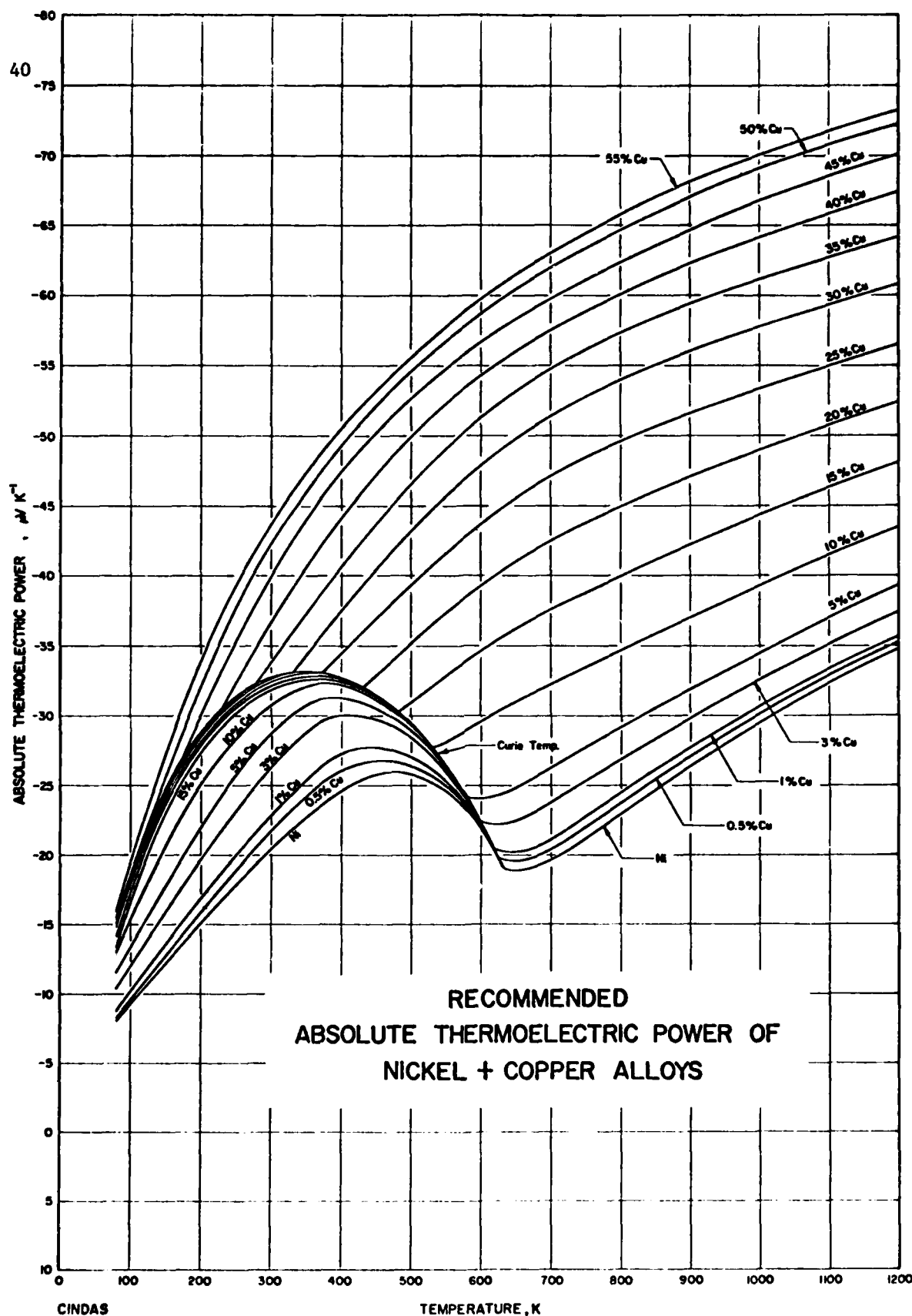


Figure 19. Recommended values for the absolute thermoelectric power of nickel + copper alloys. These recommended values were generated through data evaluation, correlation, analysis, and synthesis from the very limited experimental raw data shown in Figure 18.

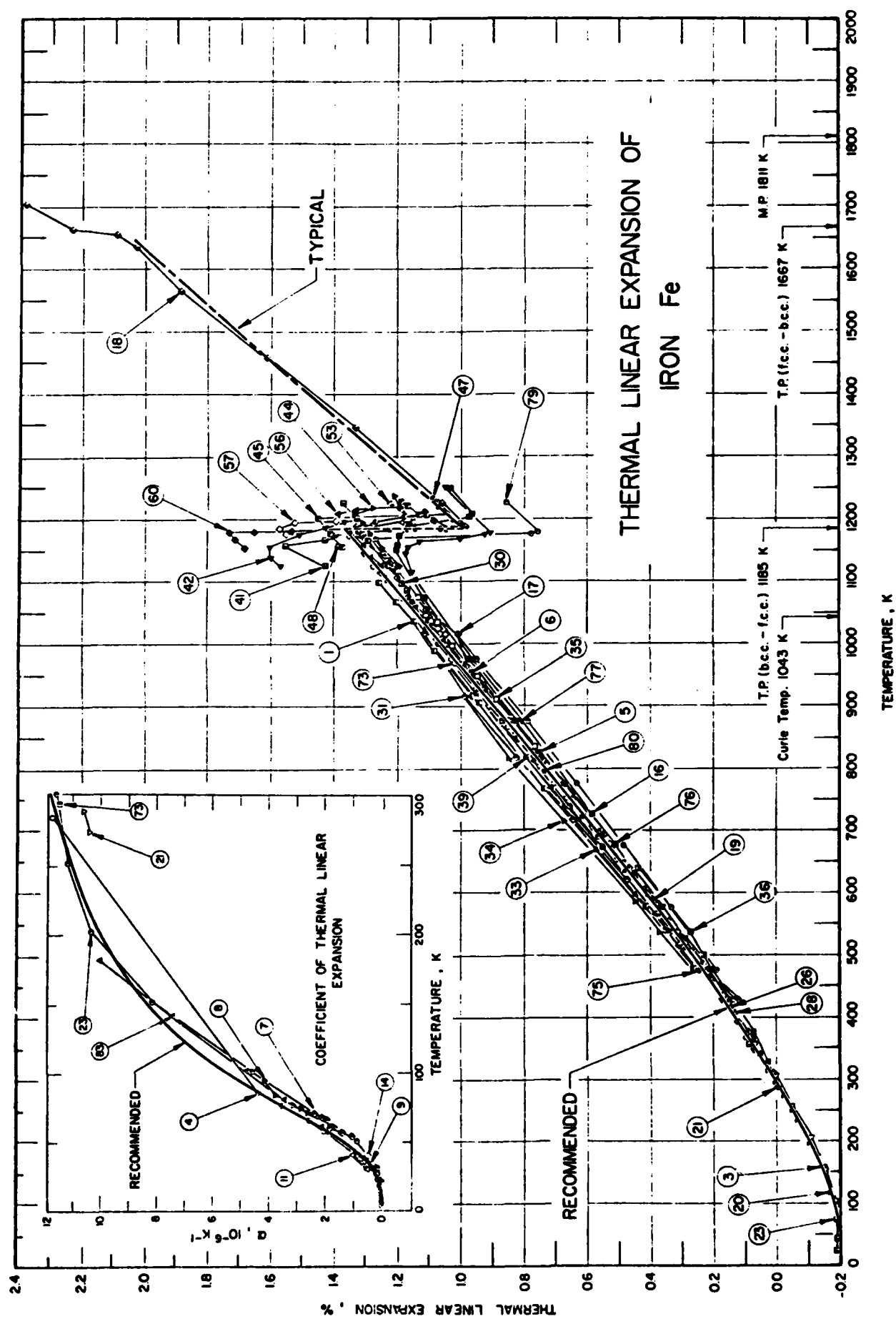


Figure 20. Experimental data and recommended values for the thermal linear expansion of iron.

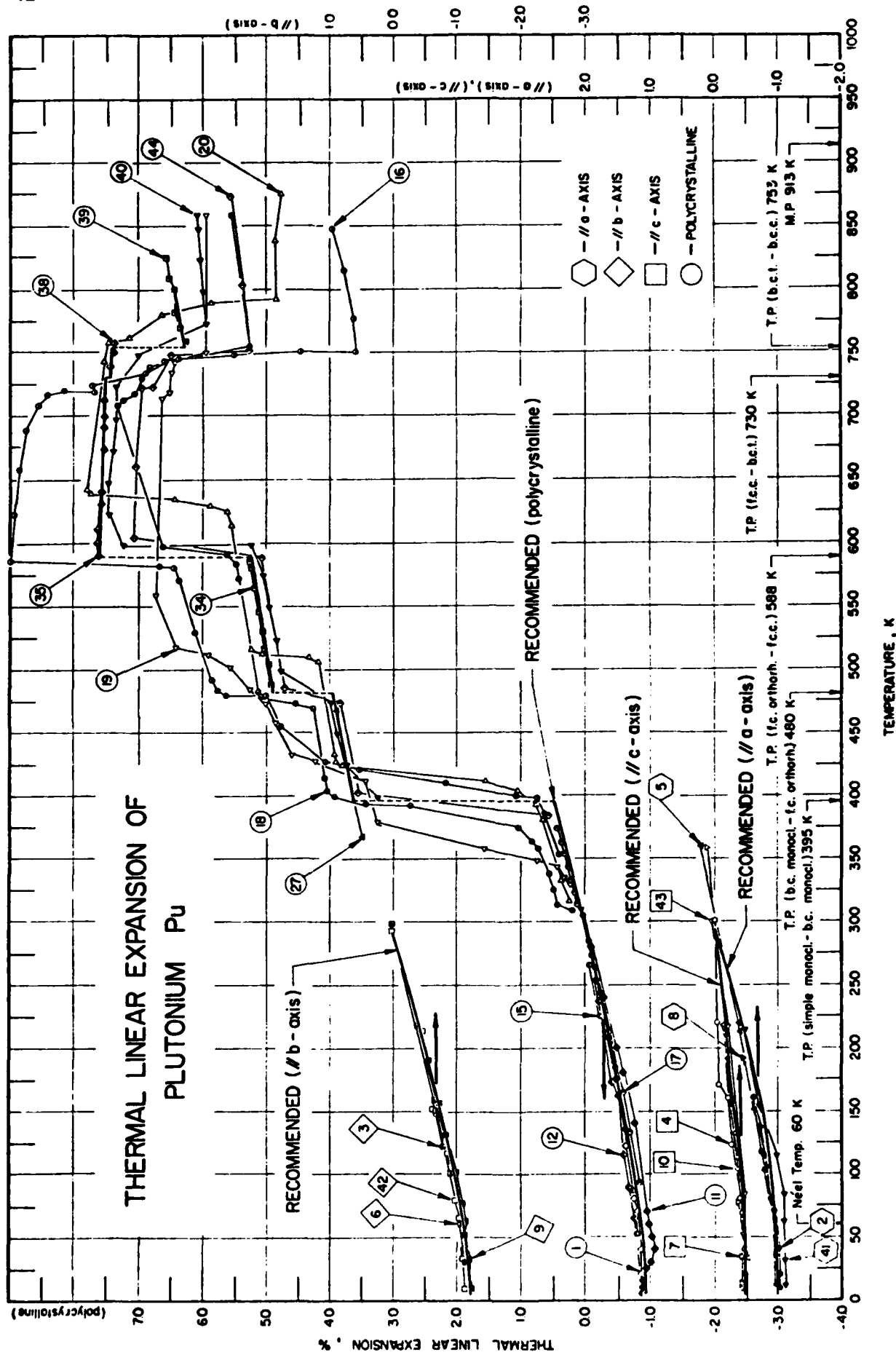


Figure 21. Experimental data and recommended values for the thermal linear expansion of plutonium.

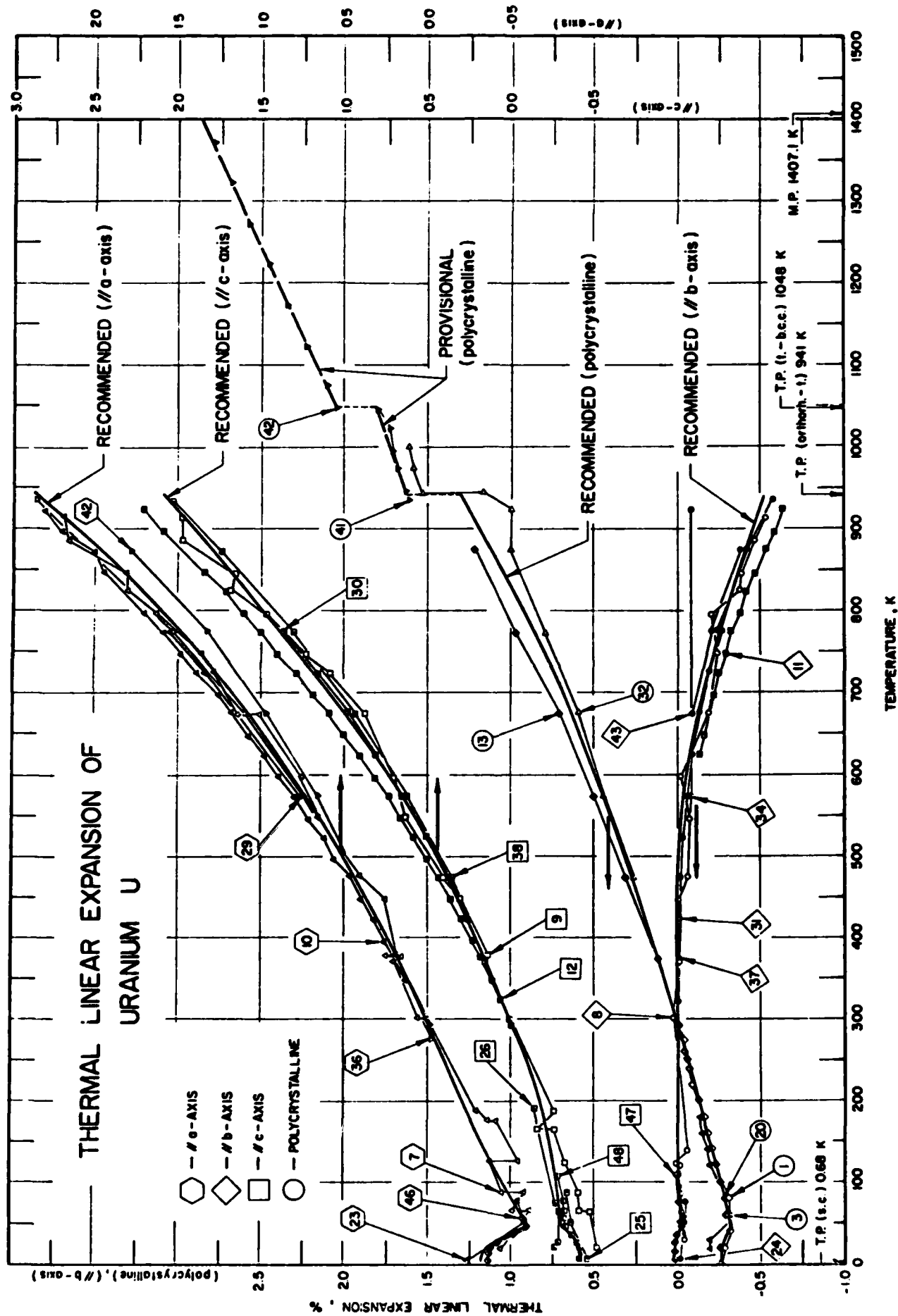


Figure 22. Experimental data and recommended values for the thermal linear expansion of uranium.

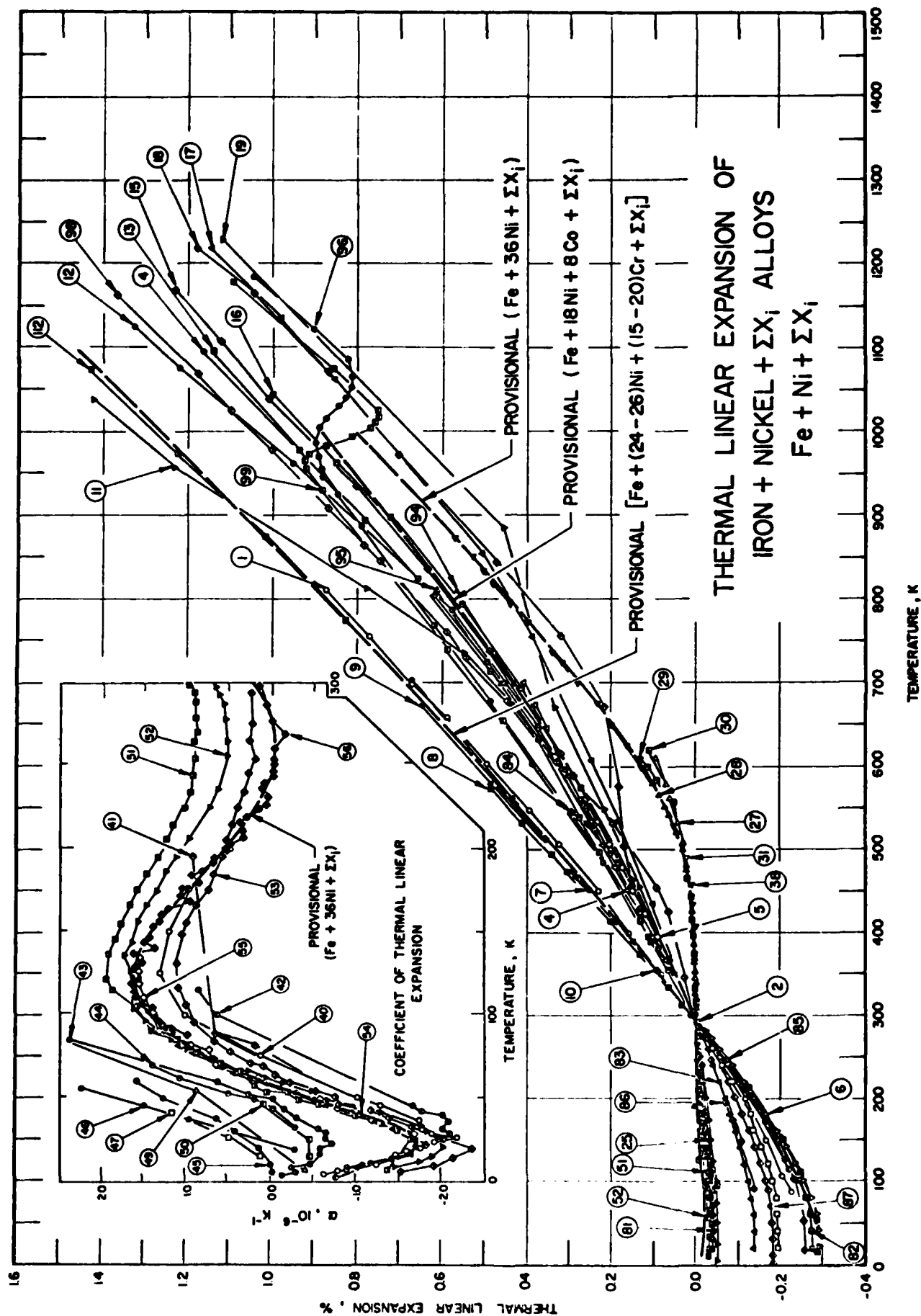


Figure 23. Experimental data and provisional values for the thermal linear expansion of nickel steels.

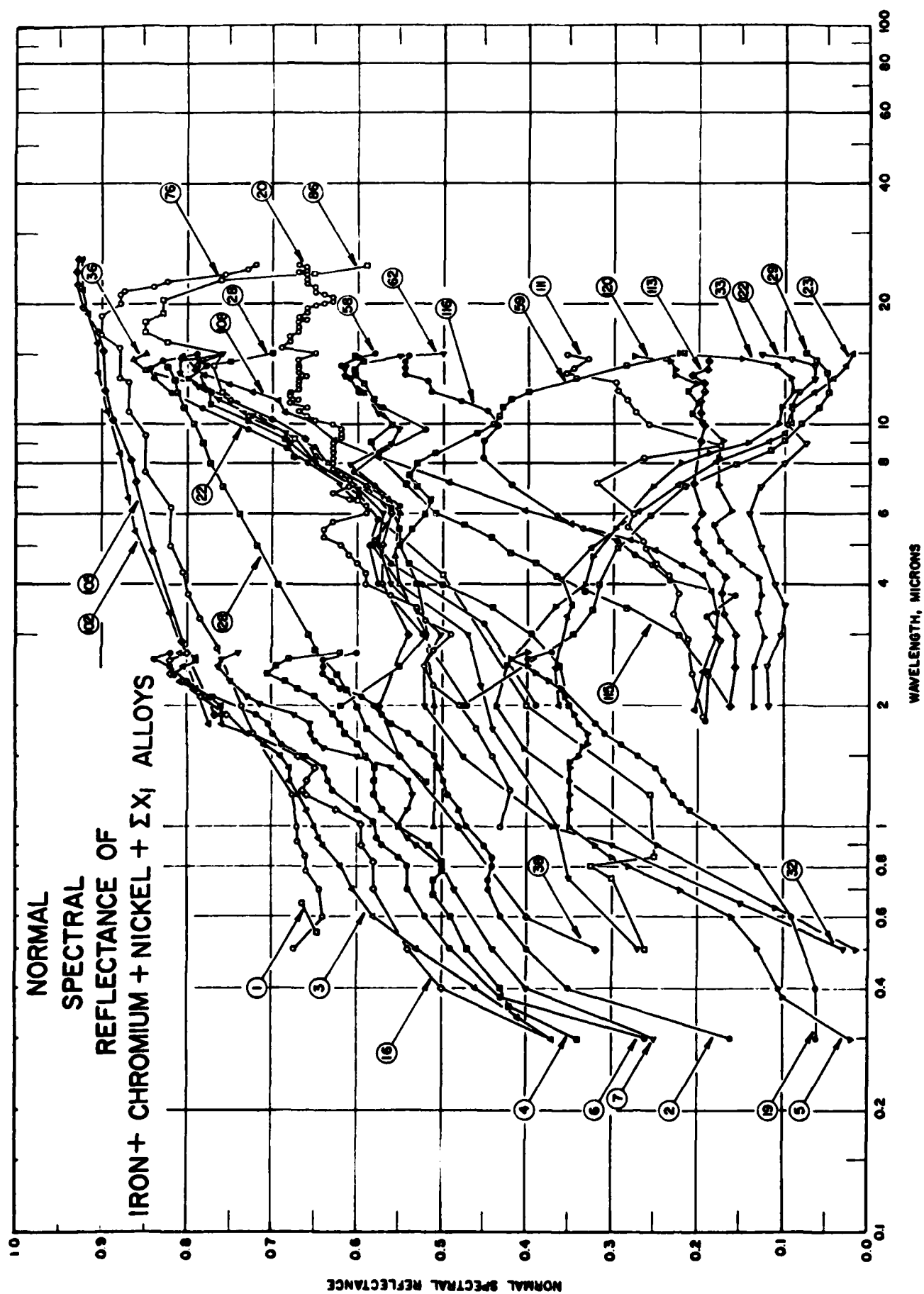


Figure 24. Experimental data on the normal spectral reflectance of stainless steels.

Figure 25. Analyzed data on the normal spectral reflectance of stainless steels.

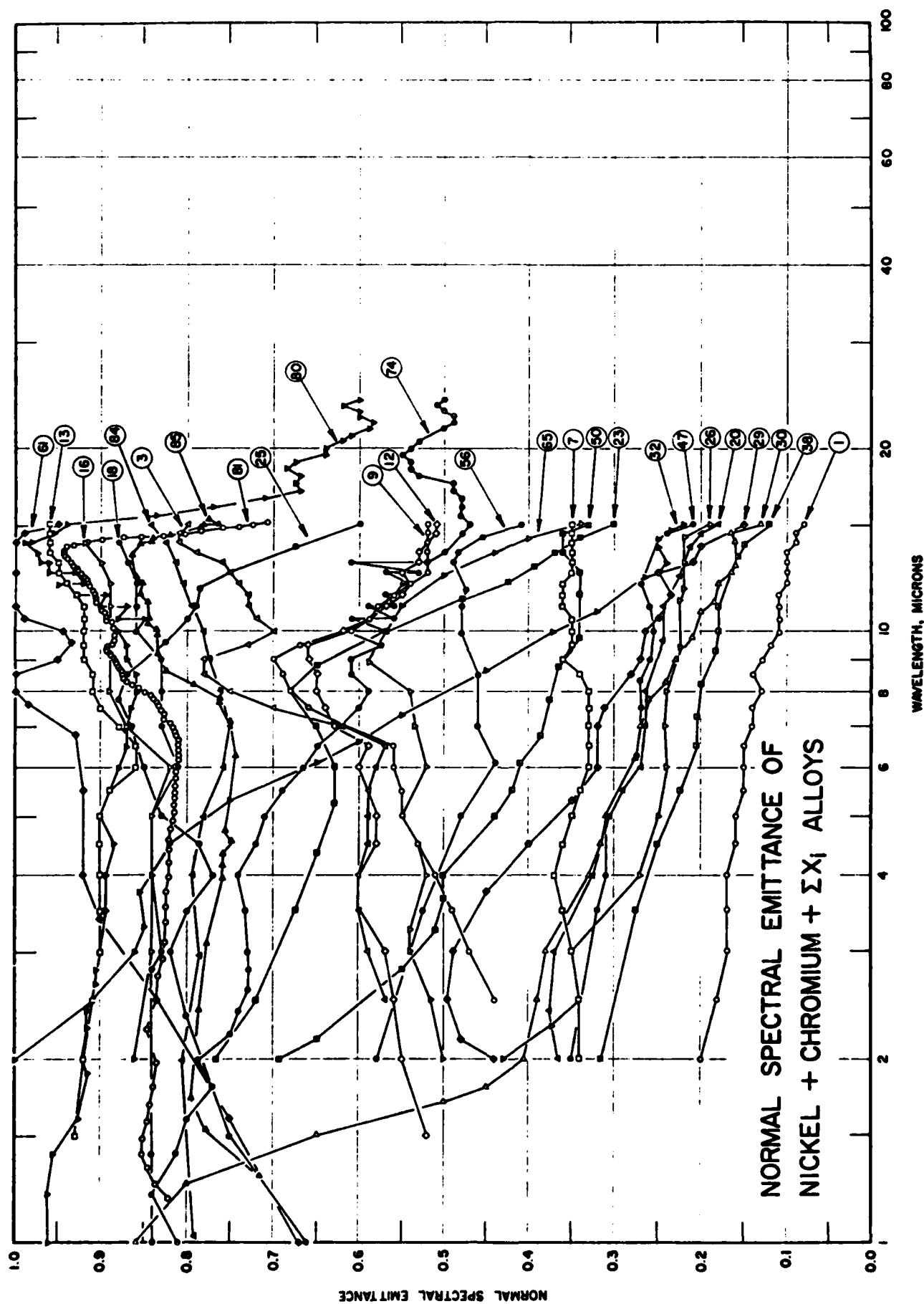


Figure 26. Experimental data on the normal spectral emittance of Inconel.

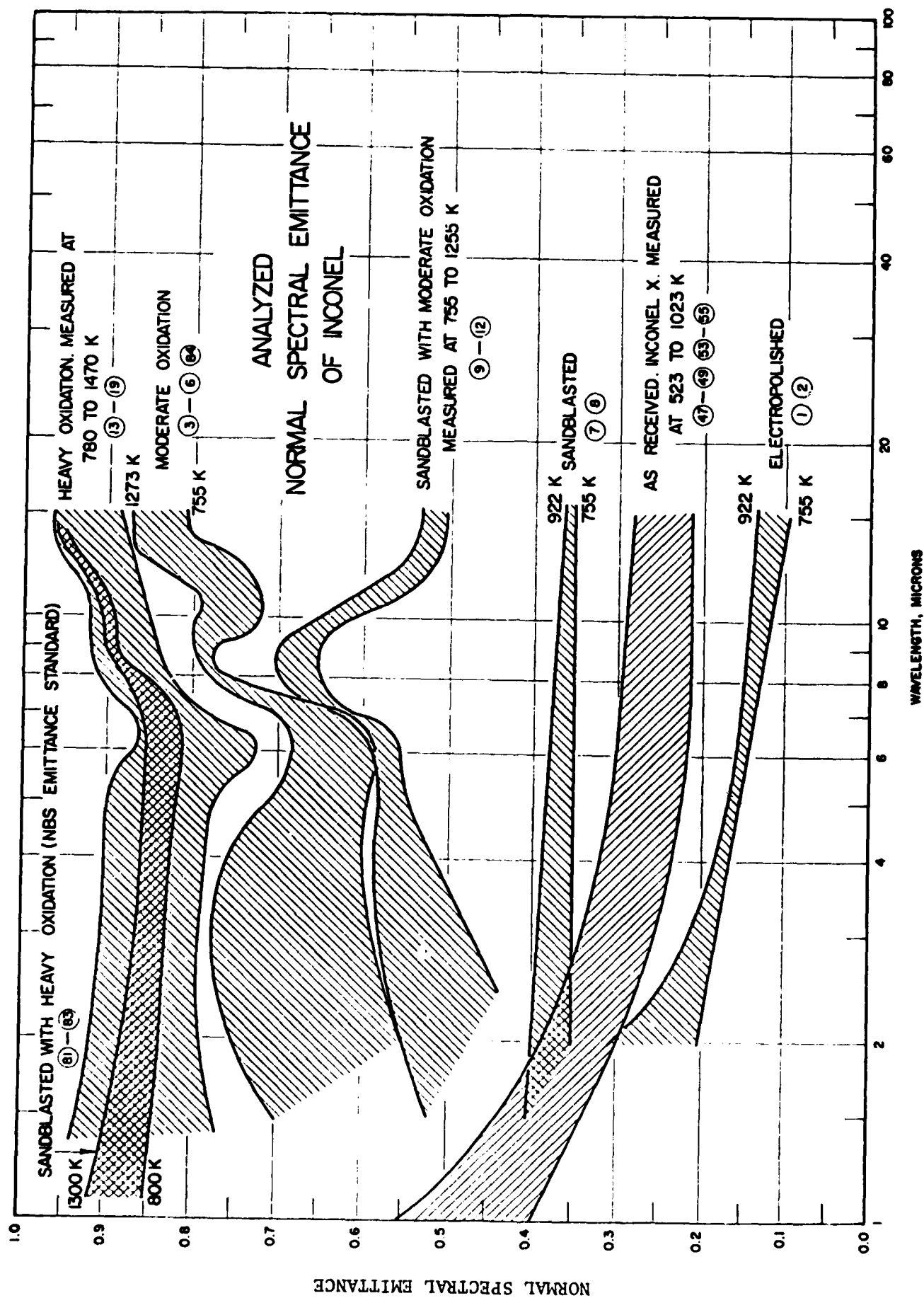


Figure 27. Analyzed data on the normal spectral emittance of Inconel.

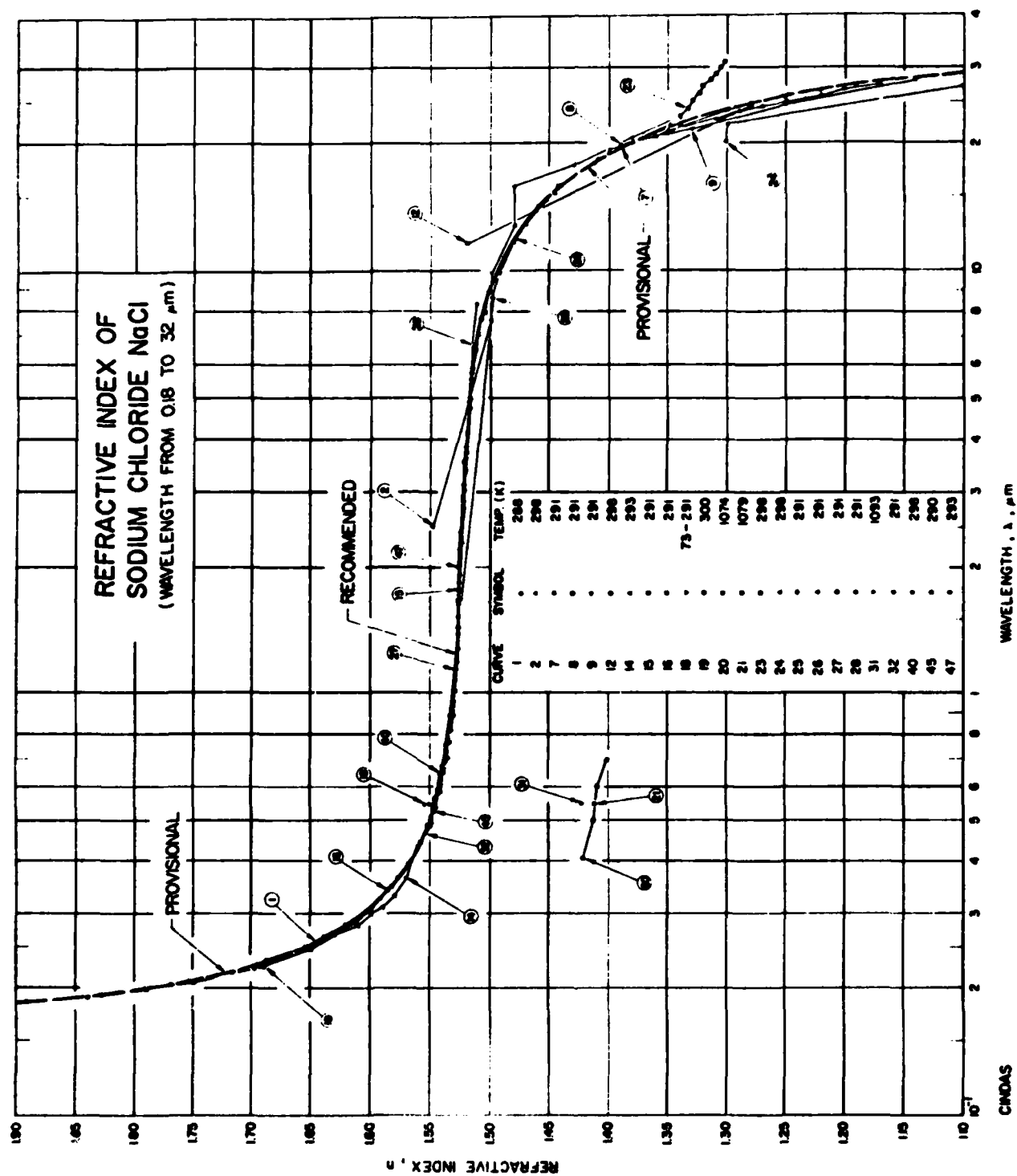


Figure 28. Experimental data and recommended and provisional values for the refractive index of sodium chloride.

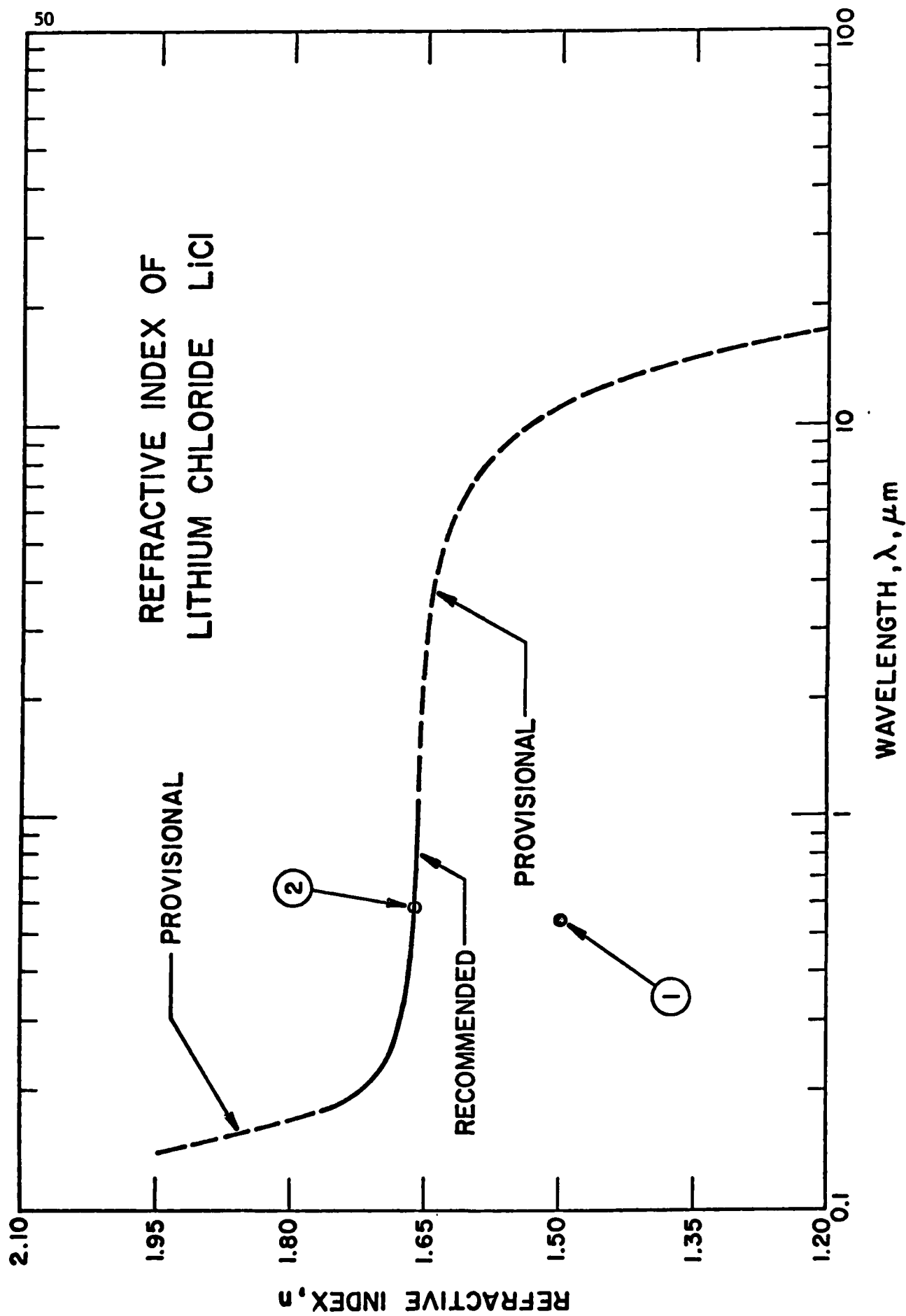


Figure 29. Experimental data and recommended and provisional values for the refractive index of lithium chloride. The lower experimental data point is far off. The full-range values are generated through data synthesis, correlation, and semi-theoretical calculation.

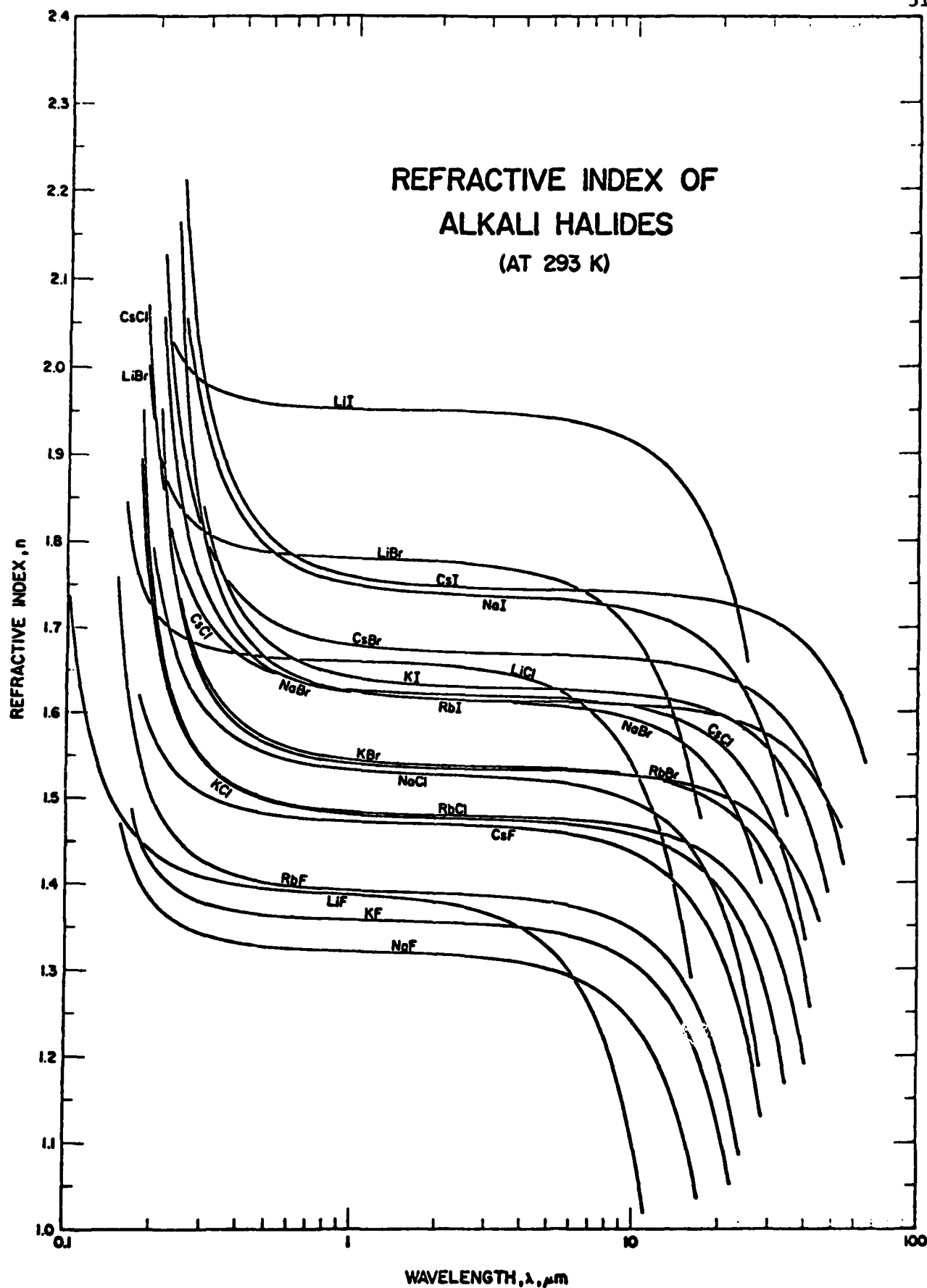


Figure 3Q Recommended and provisional values for the refractive index of all twenty alkali halides. Most of the values are generated through synthesis, correlation, prediction, and calculation.

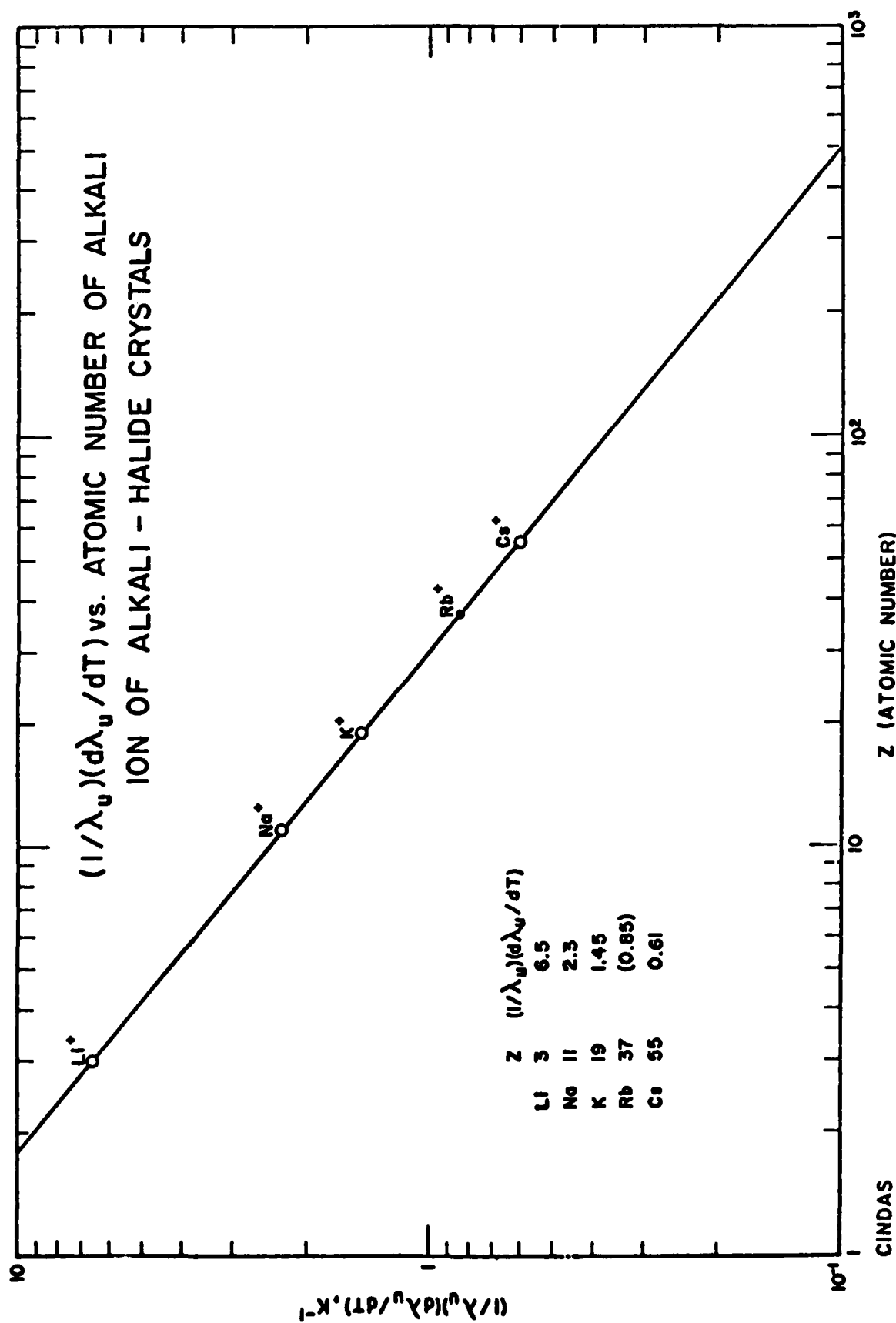


Figure 31. $(1/\lambda_u)(d\lambda_u/dT)$ versus atomic number of alkali ion of alkali-halide crystals.

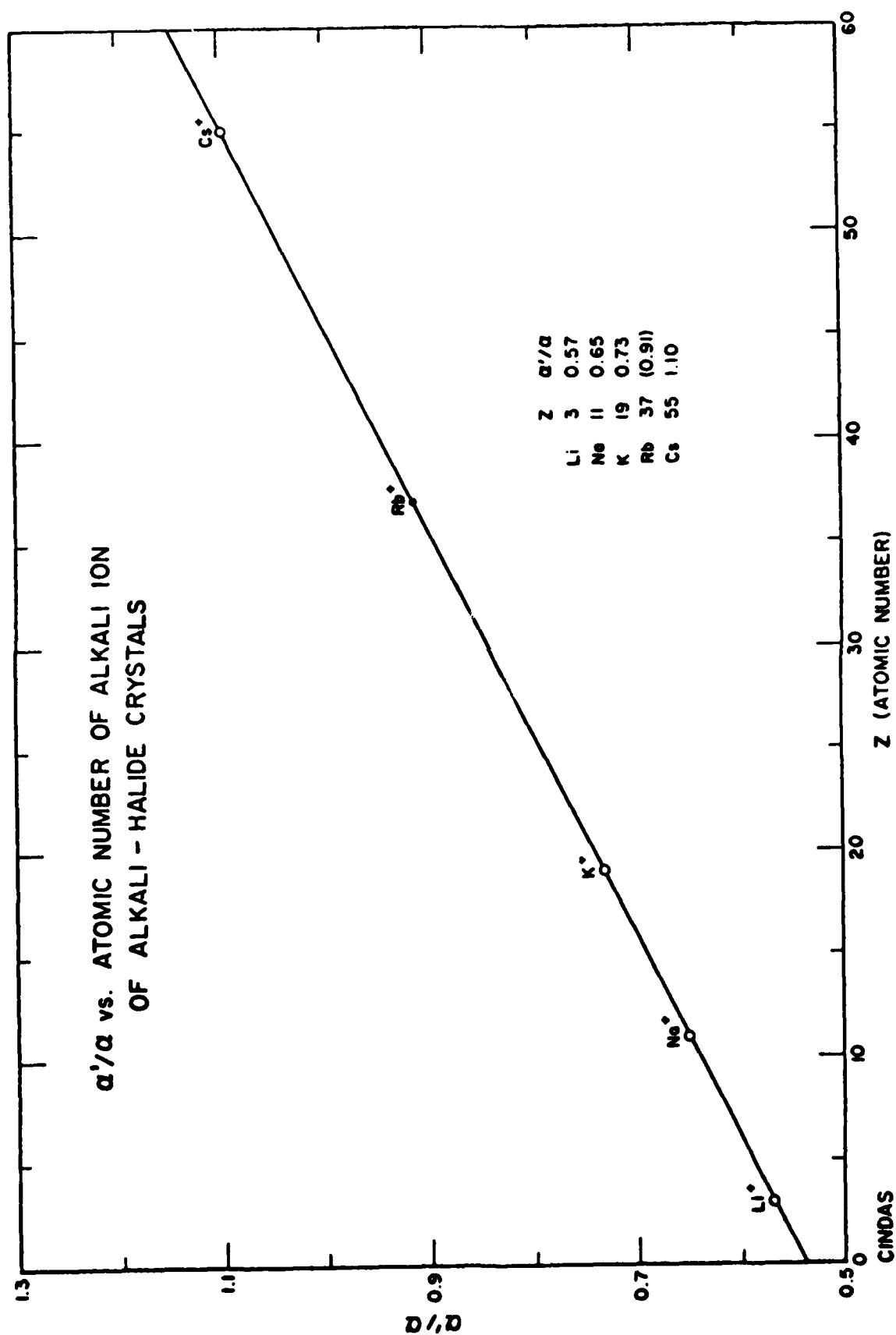


Figure 32. α'/α versus atomic number of alkali ion of alkali-halide crystals.

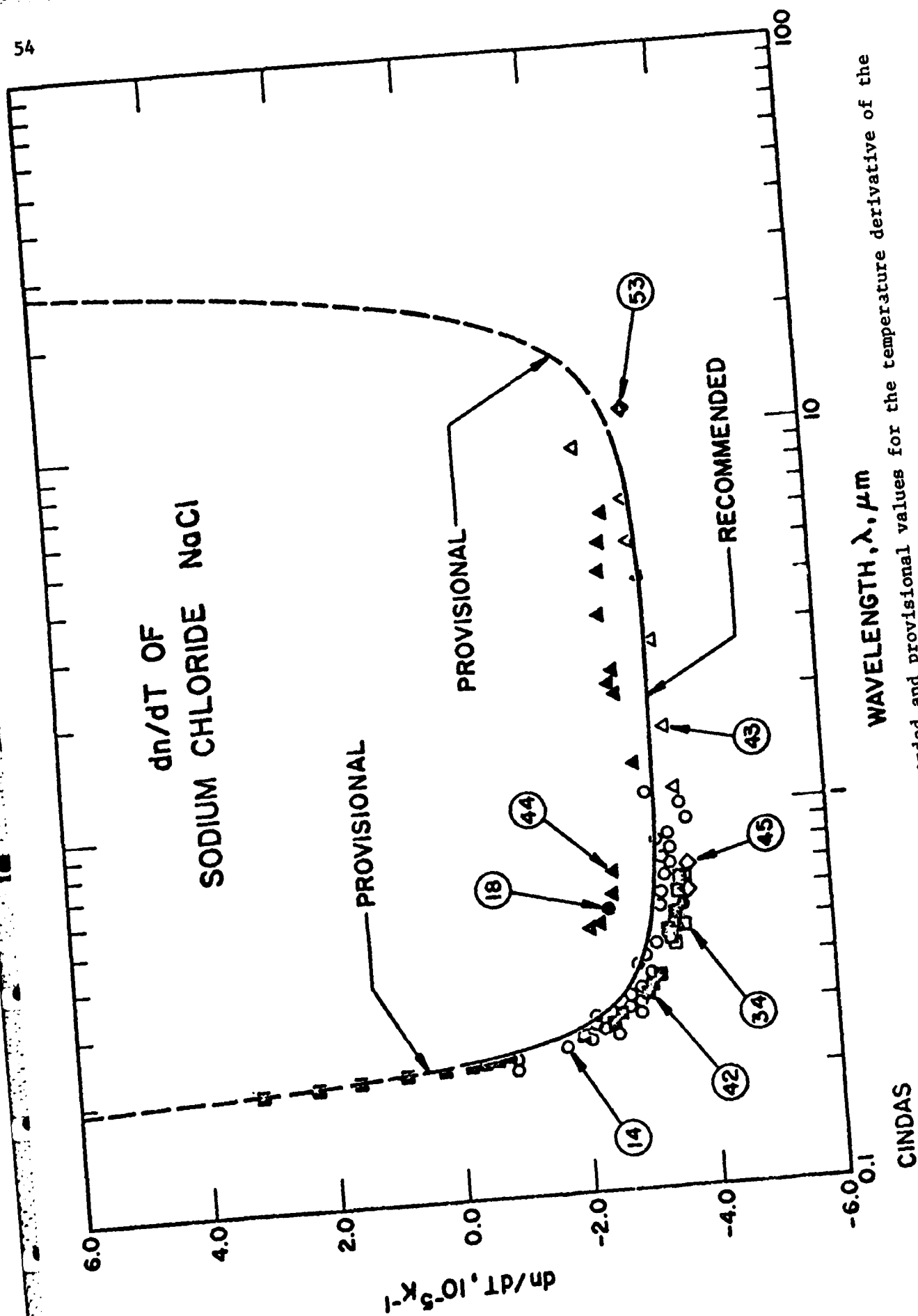


Figure 33. Experimental data and recommended and provisional values for the temperature derivative of the refractive index of sodium chloride.

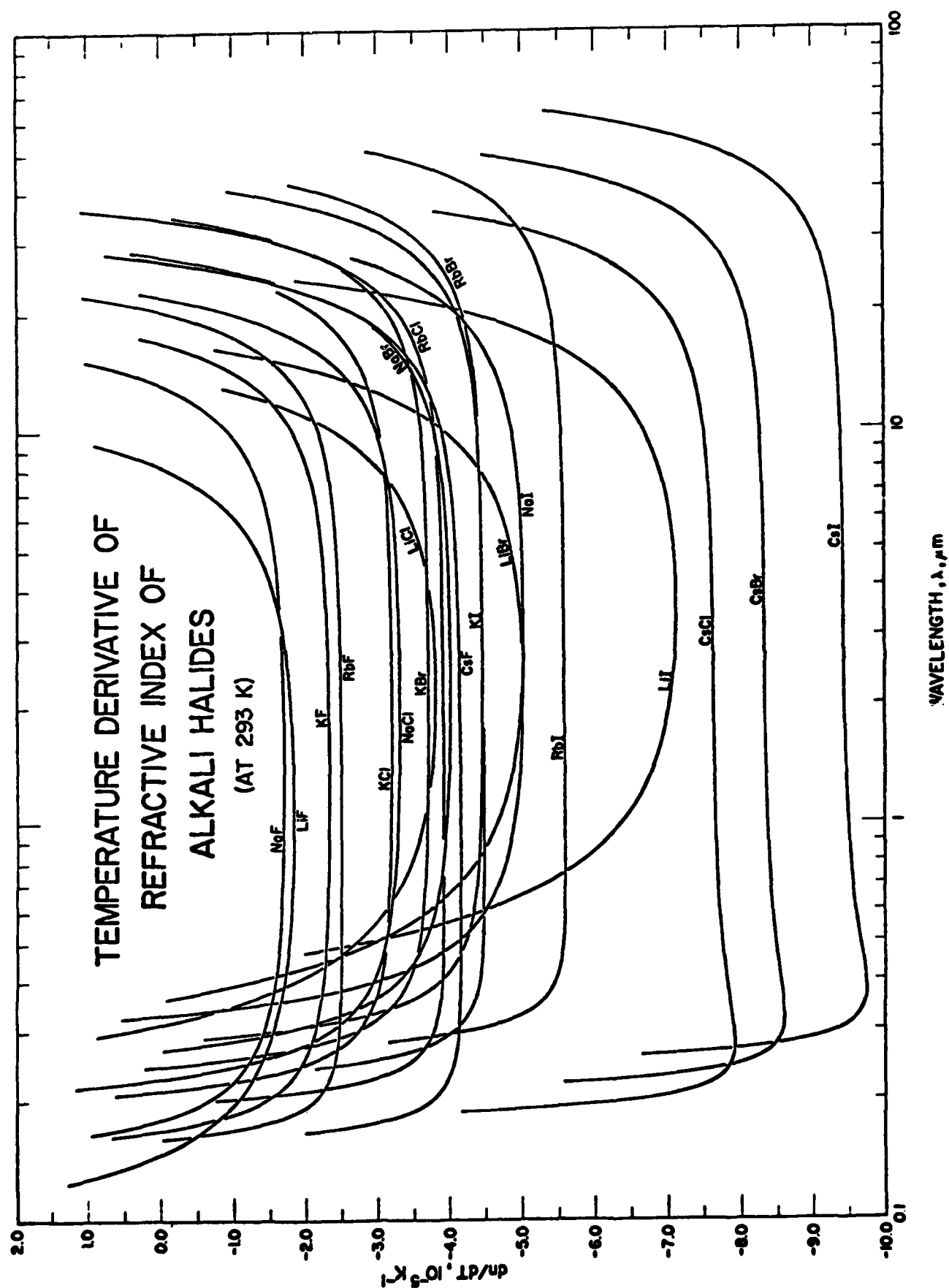


Figure 34. Recommended and provisional values for the temperature derivative of the refractive index of all twenty alkali halides. Most of the values are generated through correlation, prediction, and calculation.

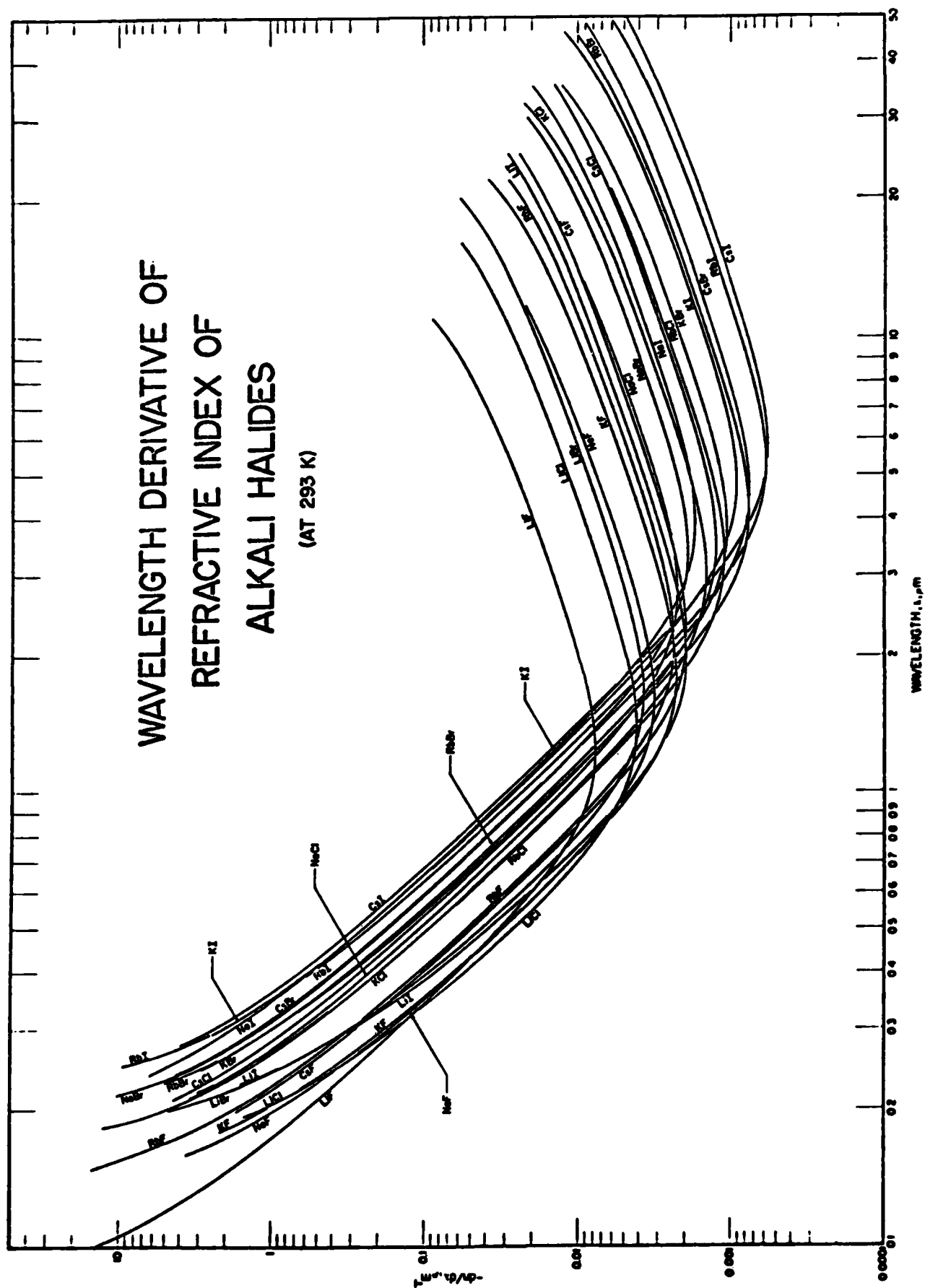


Figure 35. Provisional values for the wavelength derivative of the refractive index of all twenty alkali halides. Most of the values are calculated.

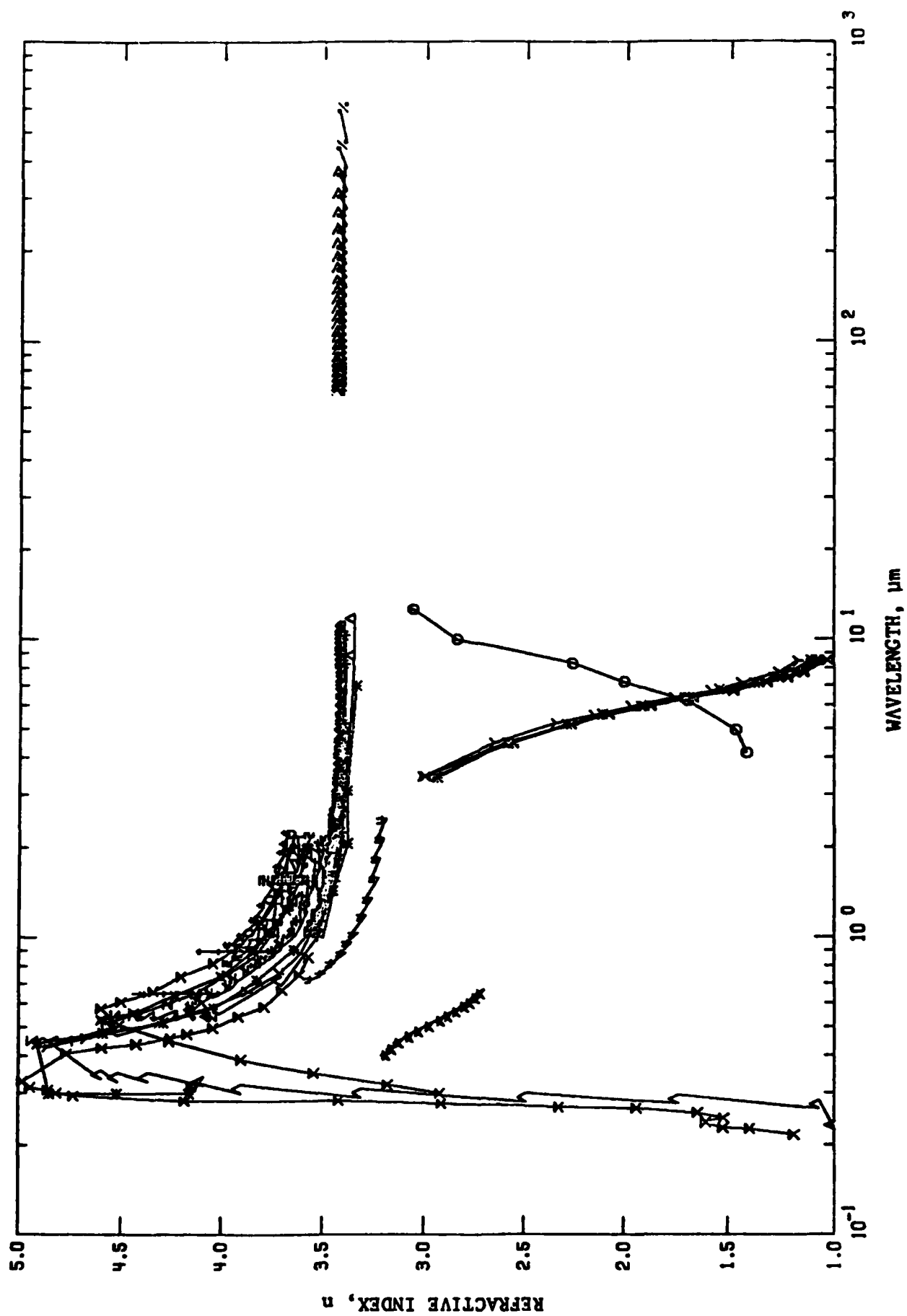


Figure 36. Experimental data on the refractive index of silicon (wavelength dependence).

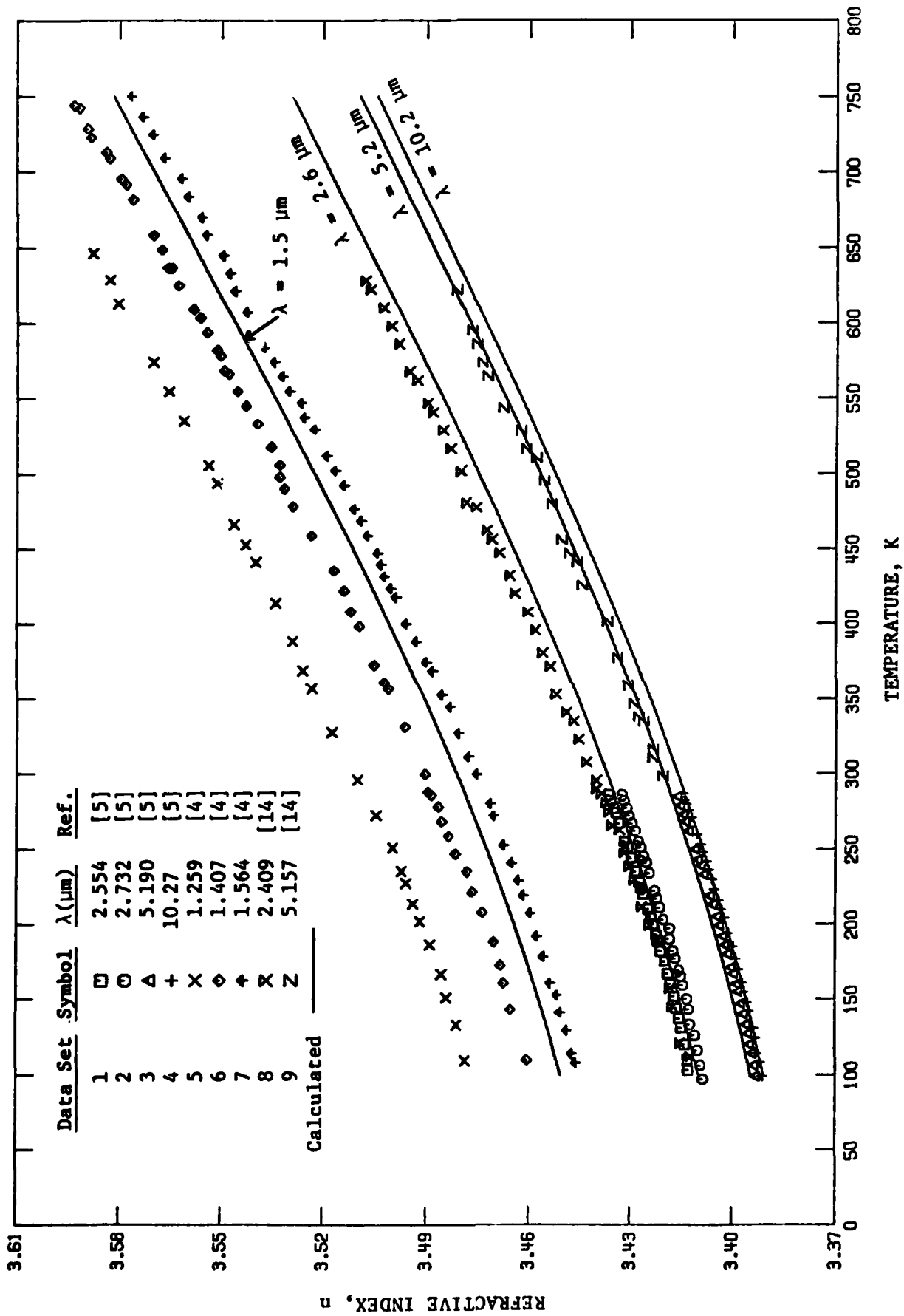


Figure 37. Experimental data on the refractive index of silicon (temperature dependence). Some calculated values are also shown for comparison.

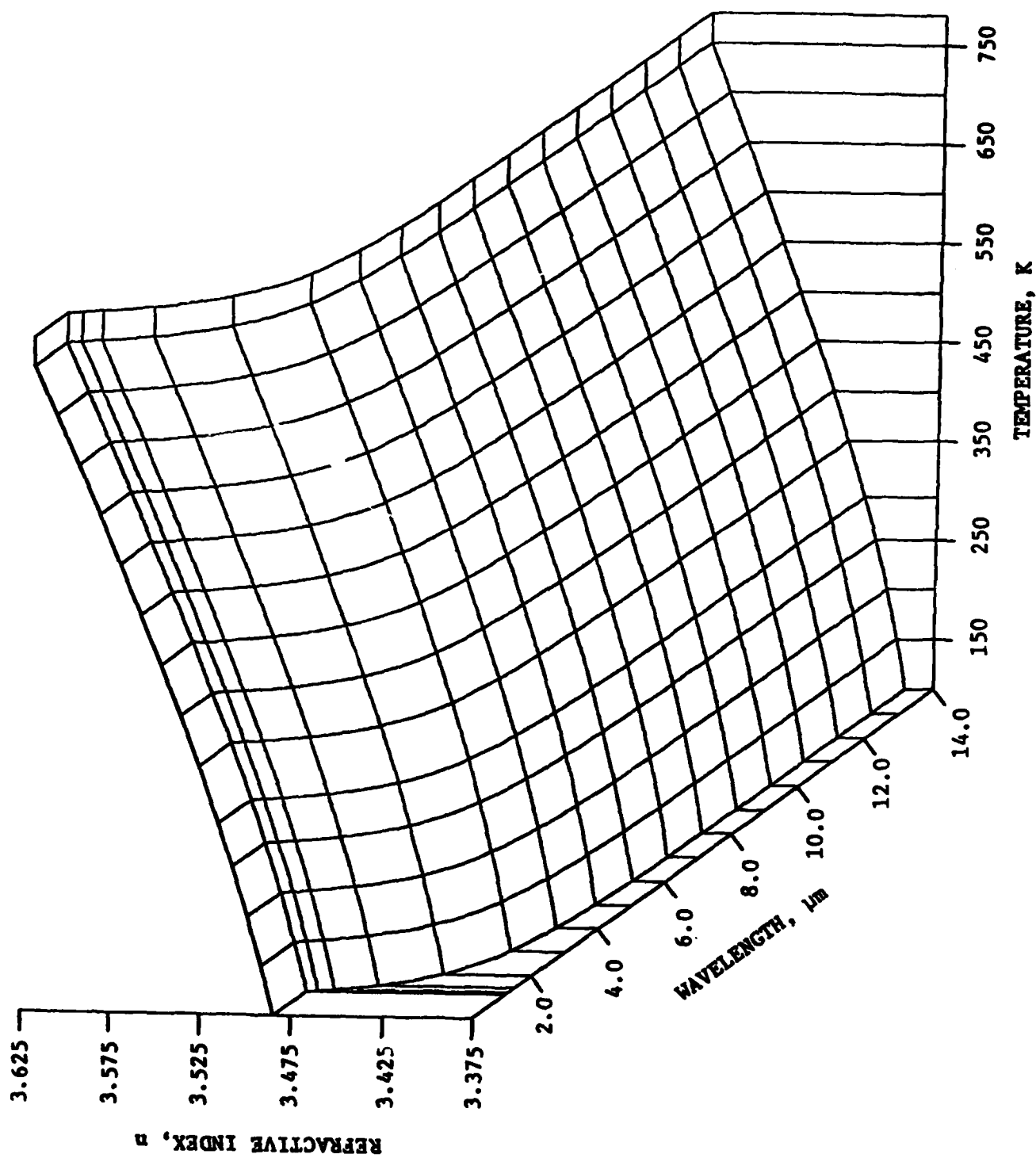


Figure 38. Recommended values for the refractive index of silicon as a function of both wavelength and temperature.

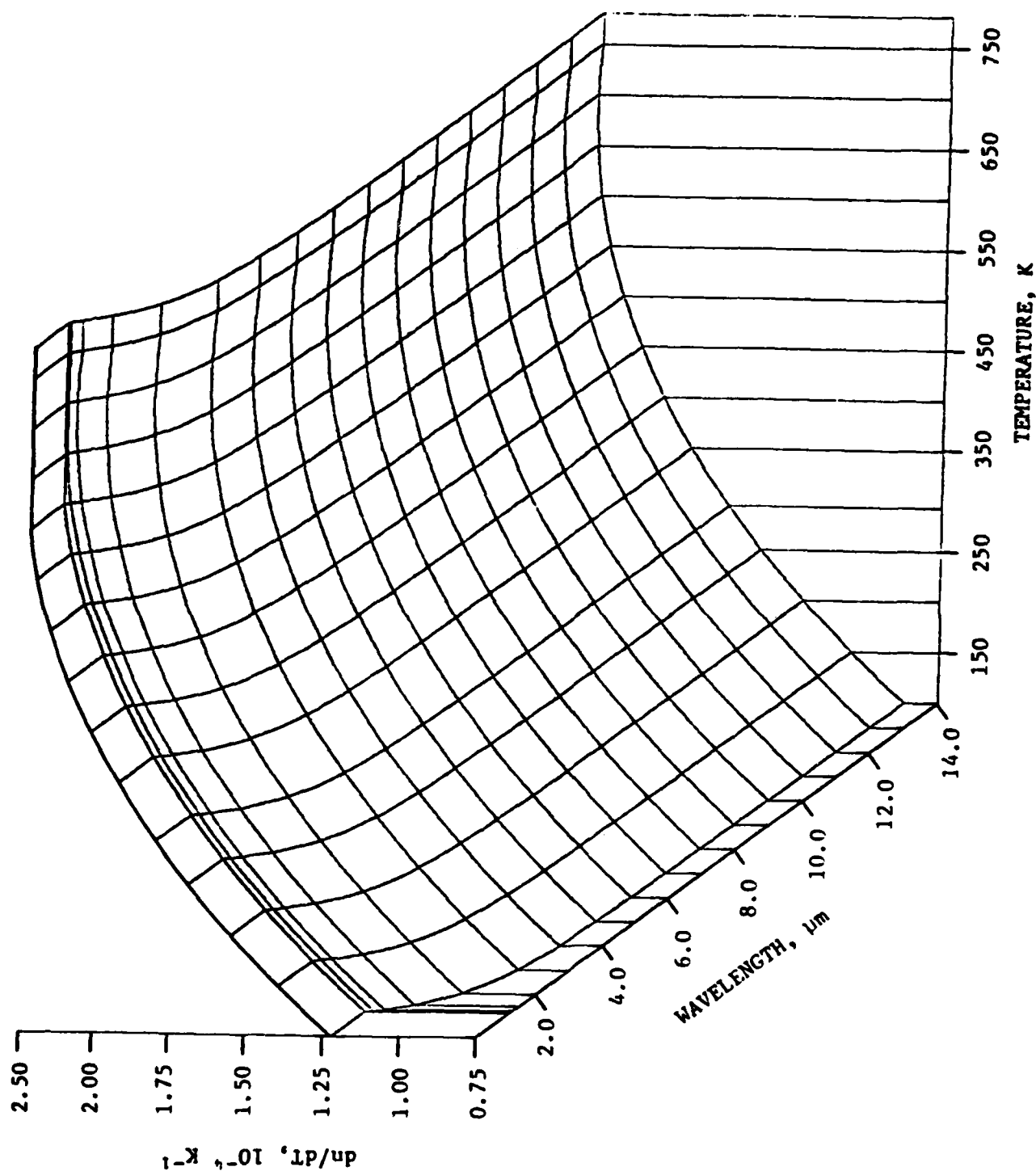


Figure 39. Recommended values for the temperature derivative of the refractive index of silicon as a function of both wavelength and temperature.

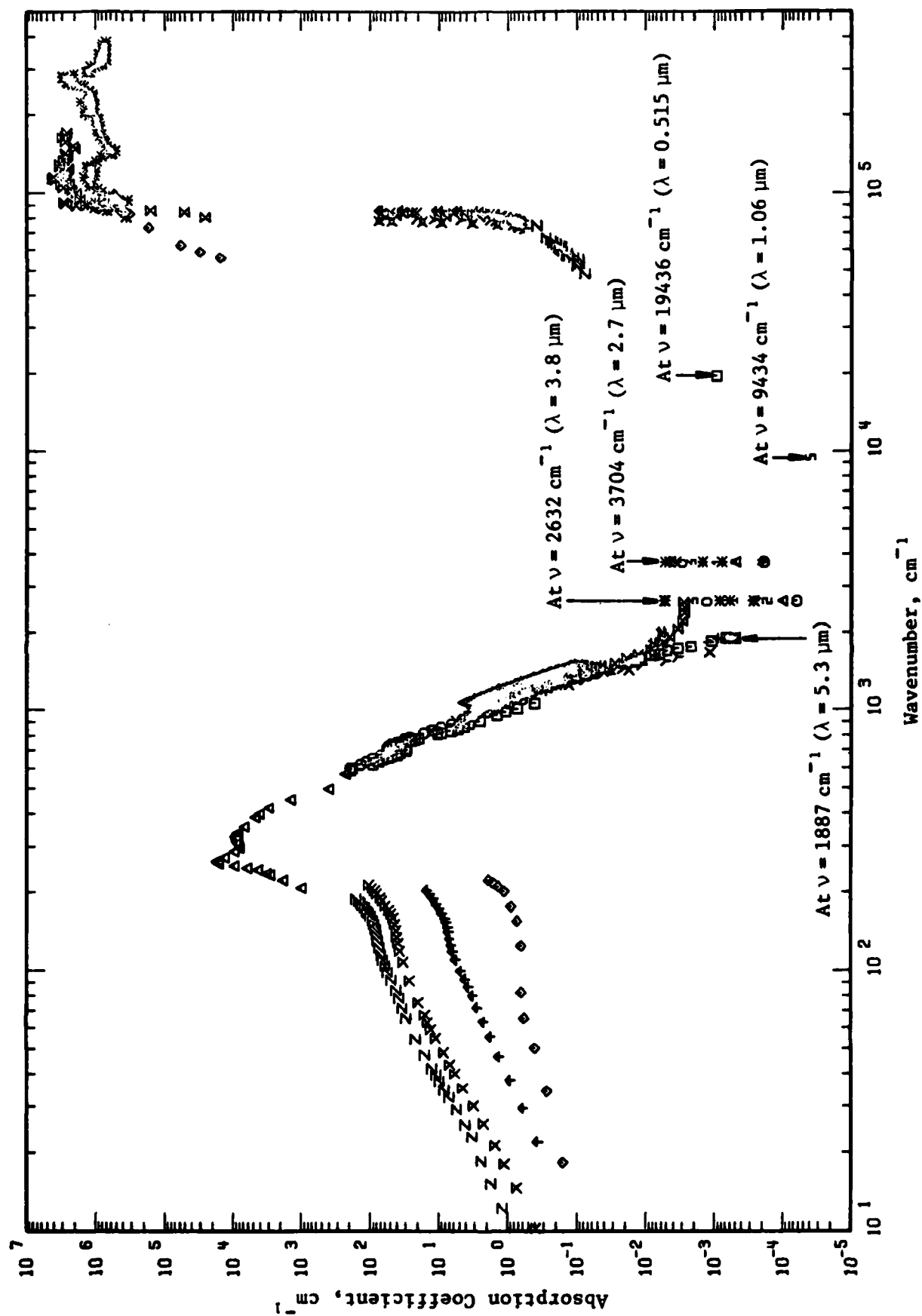


Figure 40. Experimental data on the absorption coefficient of calcium fluoride (Wavenumber Dependence).

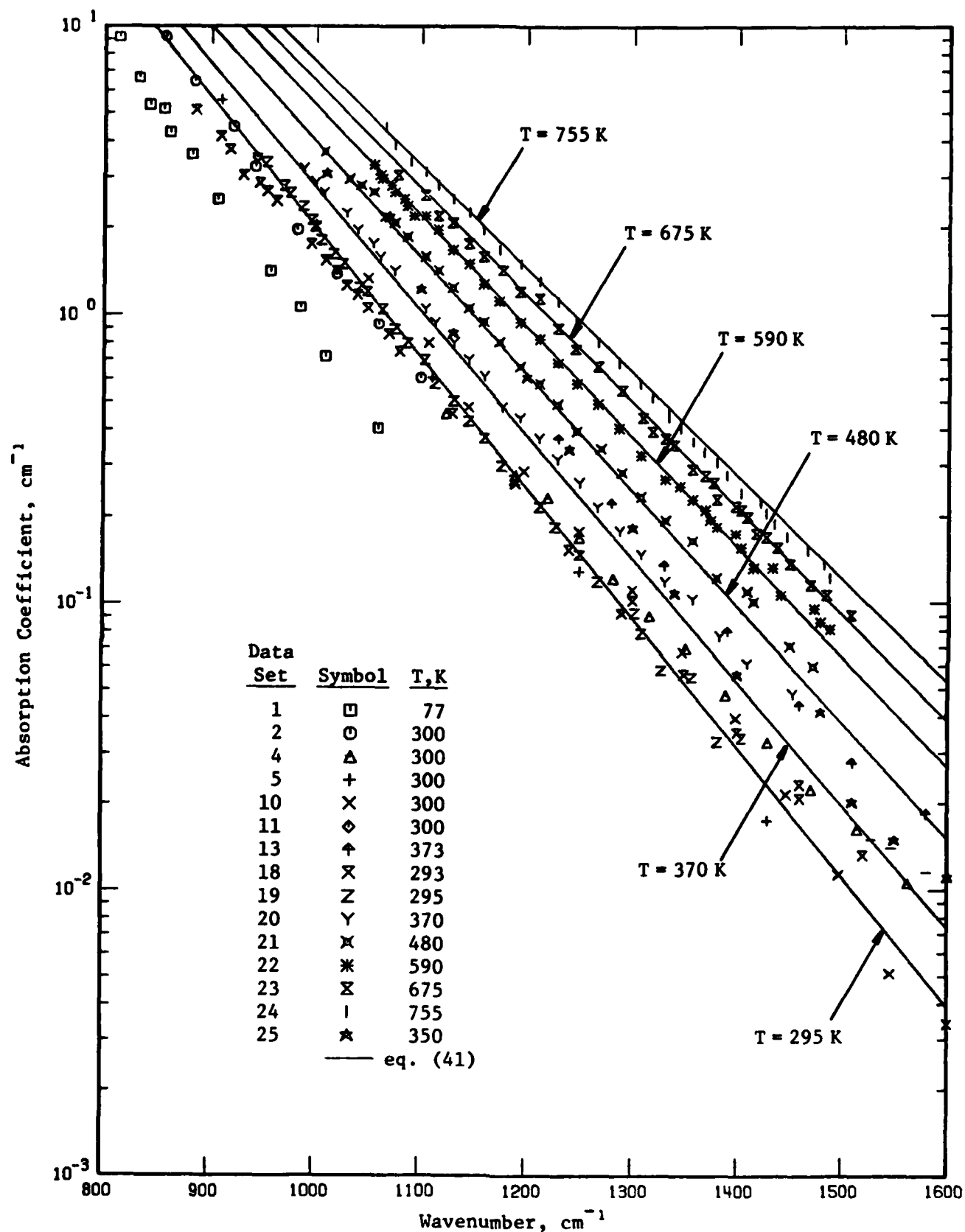


Figure 41. Experimental data on the absorption coefficient of calcium fluoride in the multiphonon region (wavenumber dependence). Some calculated values are also shown for comparison.

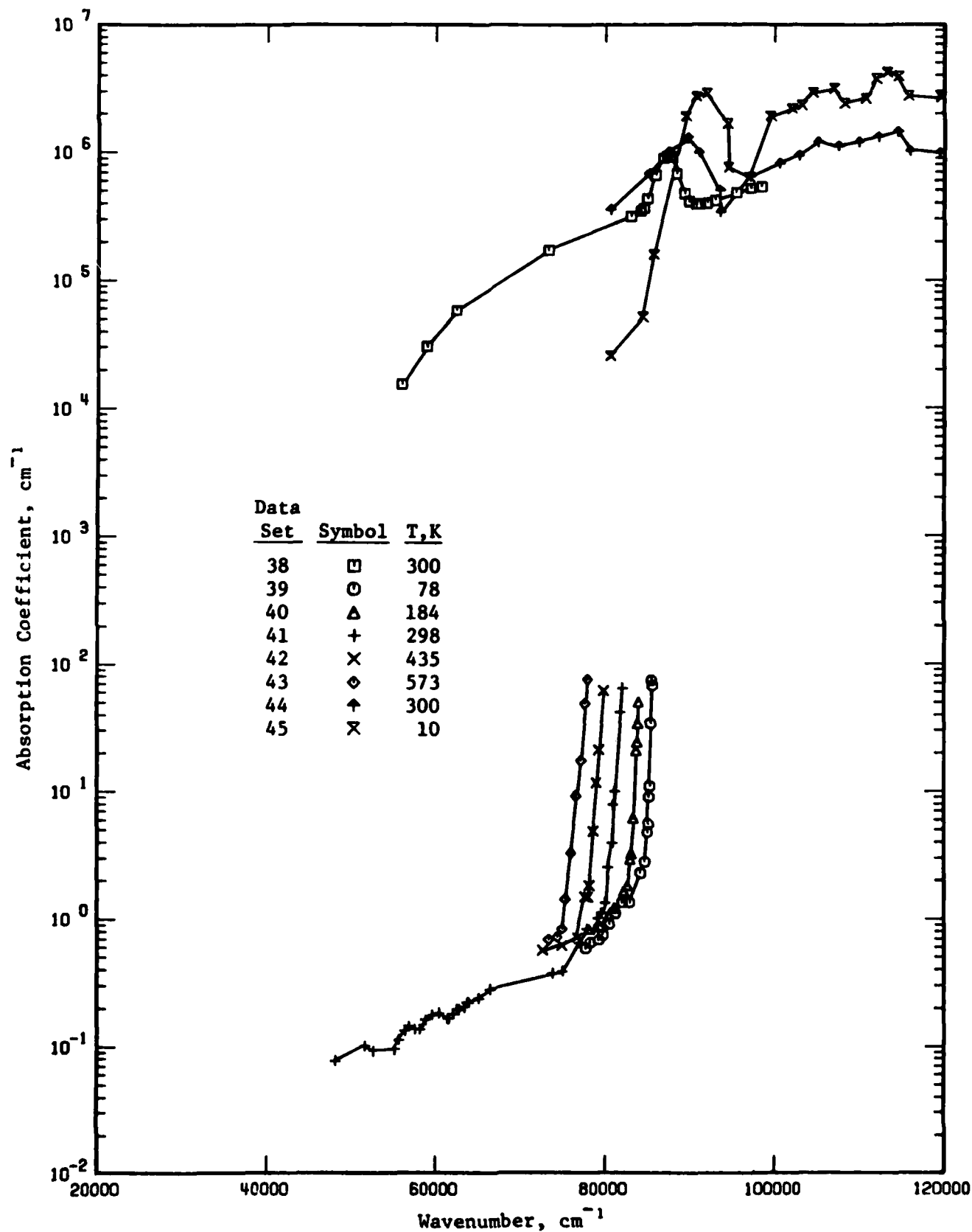


Figure 42. Experimental data on the absorption coefficient of calcium fluoride in the Urbach tail region (wavenumber dependence).

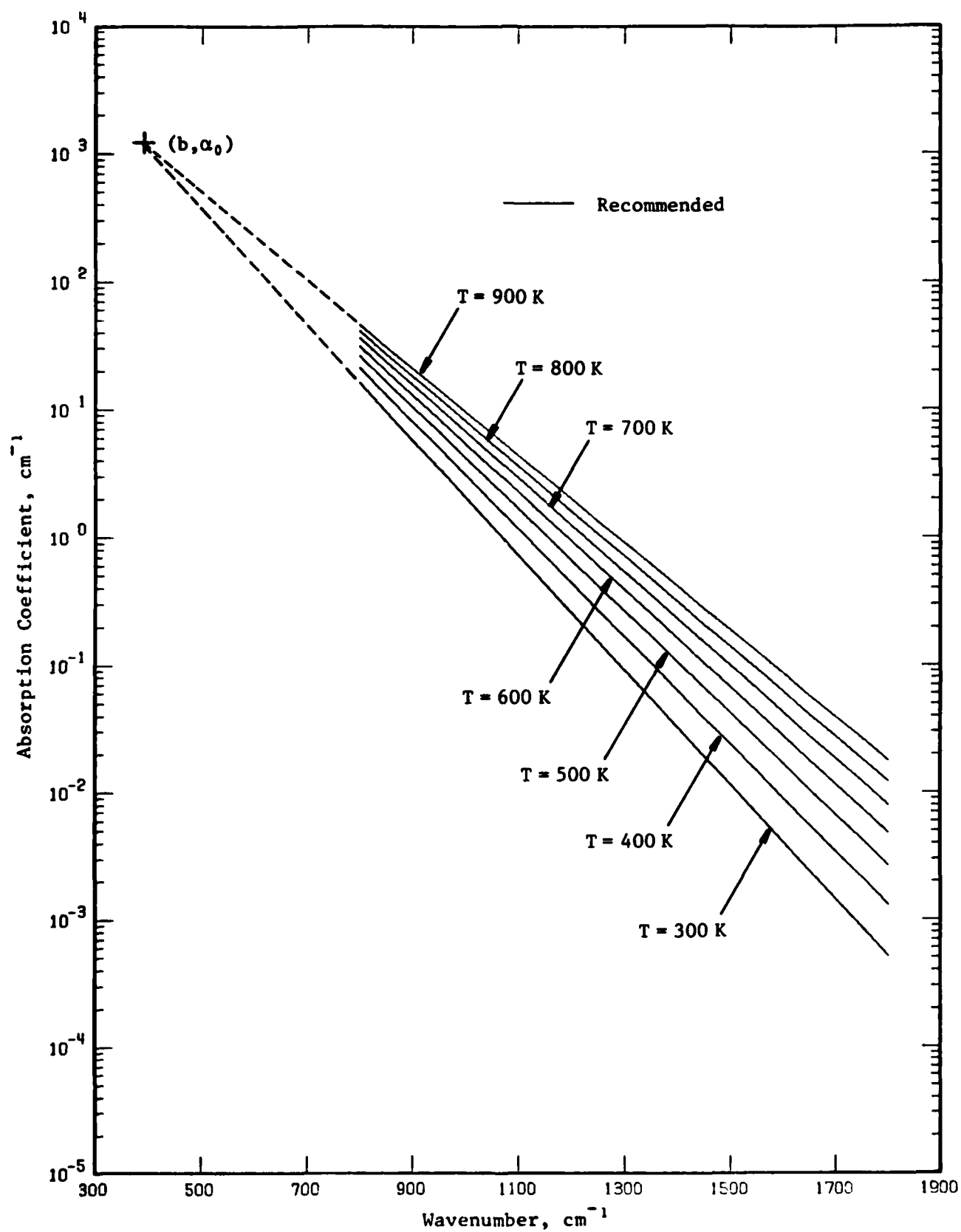


Figure 43. Recommended values for the absorption coefficient of calcium fluoride (wavenumber dependence).

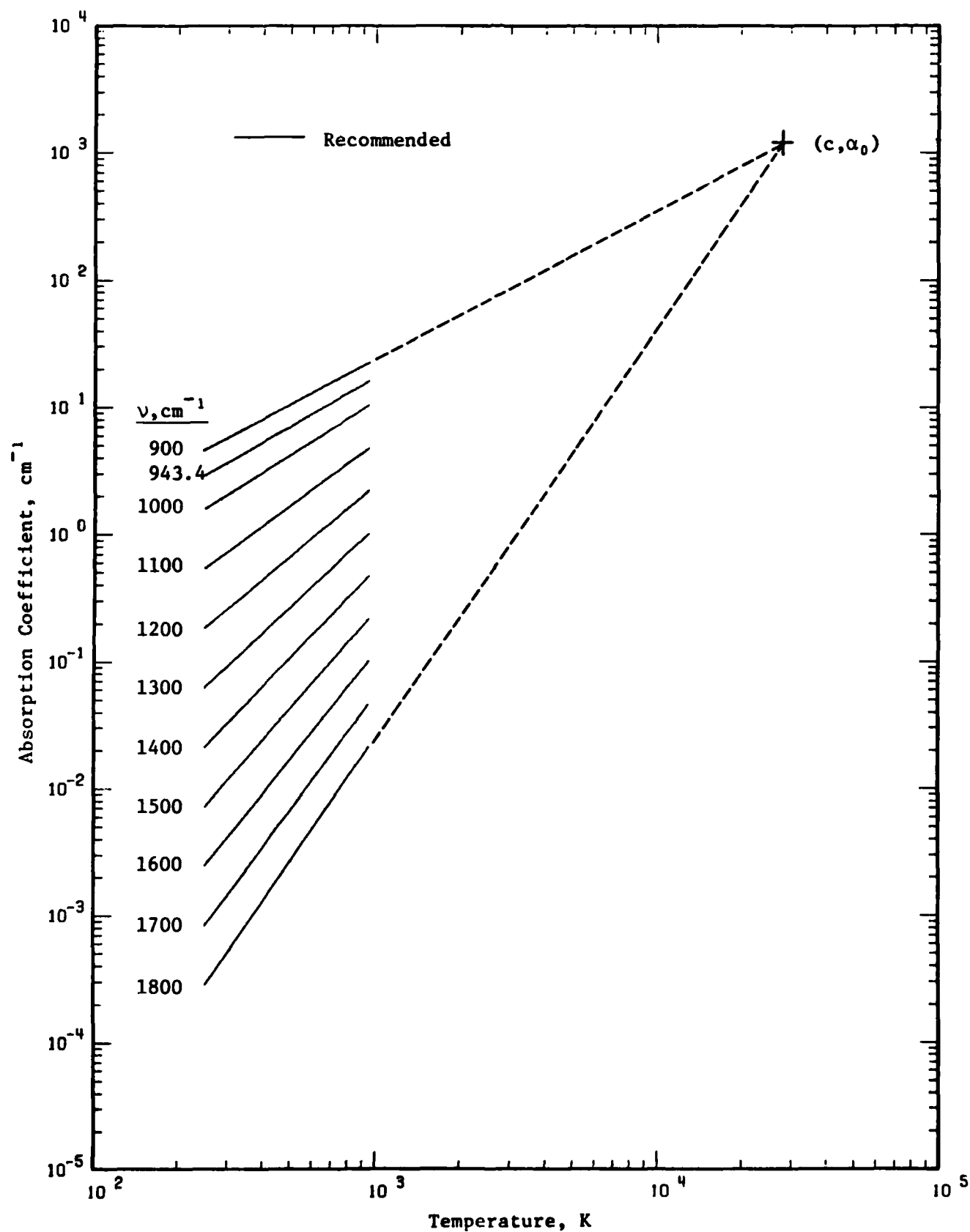


Figure 44. Recommended values for the absorption coefficient of calcium fluoride (temperature dependence).

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The methodology of critical evaluation, correlation, analysis, and synthesis of physical properties data used at the Thermophysical and Electronic Properties Information Analysis Center (TEPIAC) of the Center for Information and Numerical Data Analysis and Synthesis (CINDAS), Purdue University, is described and discussed, and further illustrated with practical examples covering thermal conductivity, thermal diffusivity, electrical resistivity, thermoelectric power, and refractive index of various solid materials. It is demonstrated that data evaluation, correlation, analysis, and synthesis is a very powerful tool that not		

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only can bring order out of conflicting, confusing, and chaotic experimental observations, but also can create new knowledge, which in itself is a major contribution to science and technology. It is shown further that critically evaluated, recommended reference data are generated at a tiny fraction of the cost and time required for producing the original experimental raw data, and that data critique must be considered an integral part of research if research results are to be meaningful and useful.

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